From particle simulations to flow models - for cohesive frictional, sintering materials

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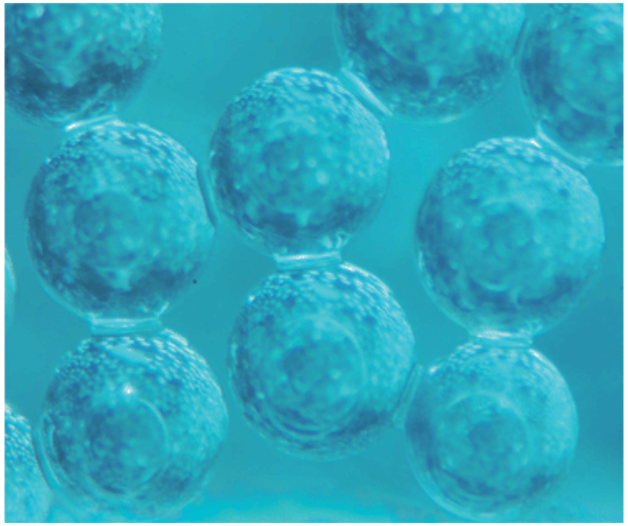
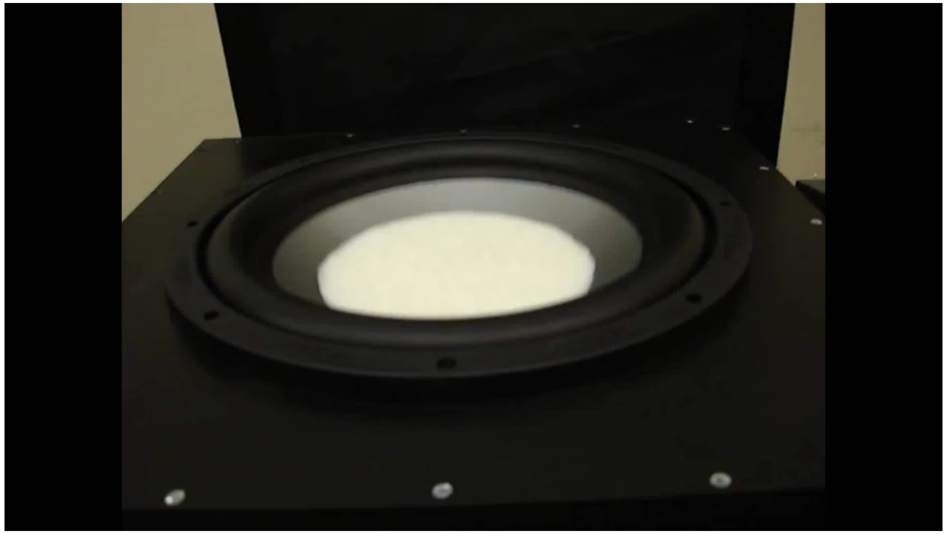
T-MAPPP Common issues

- From micro/contact-mechanics to macro-behaviour
- Calibration and Validation
- Choice of calibration tests and relevant parameters - depending on (flow) regime(s) and application.
- CPU-time when running moderate to large DEM
- Apply modern and novel experimental techniques for additional information not available otherwise

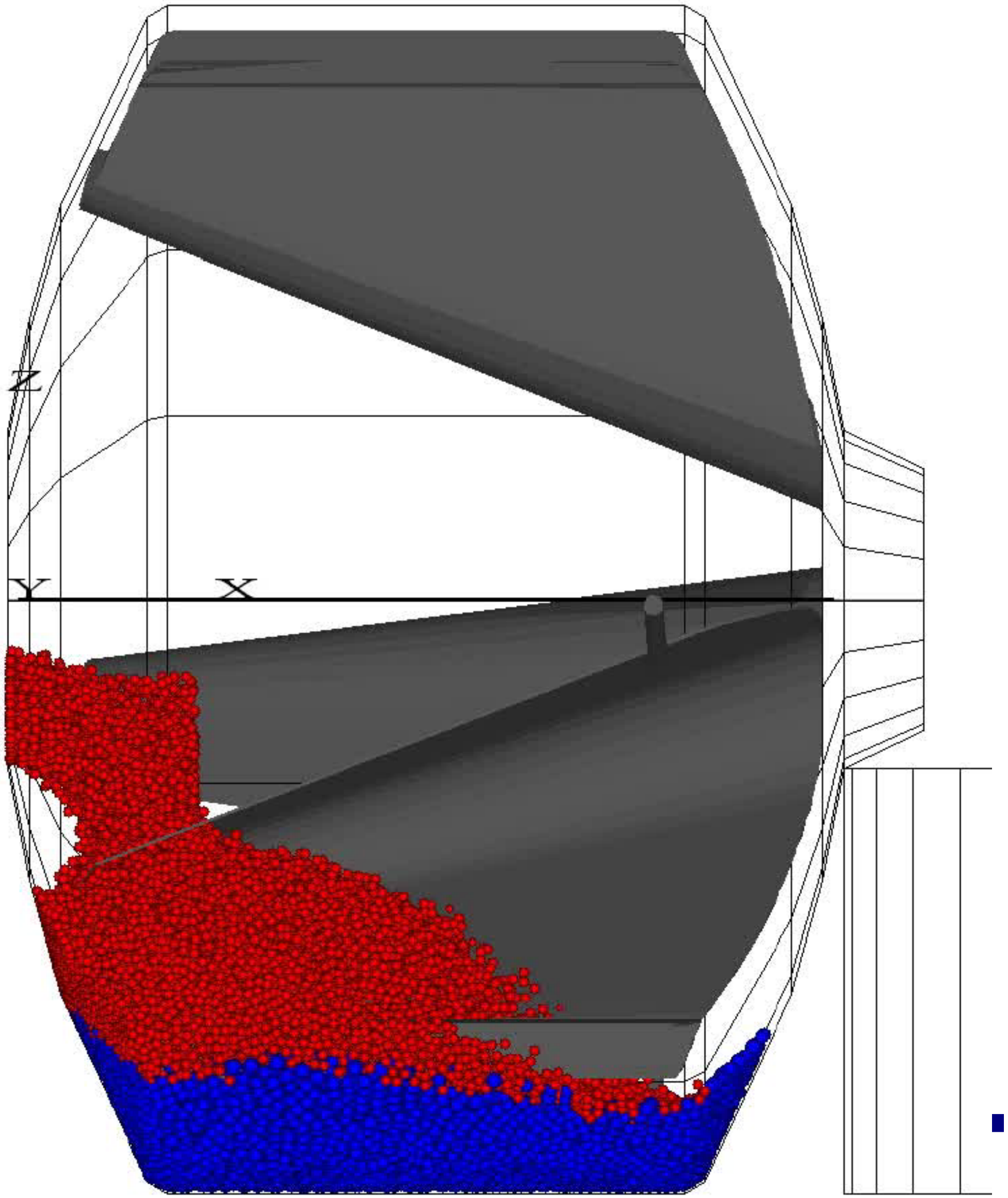
Packing:

micro-structure + history



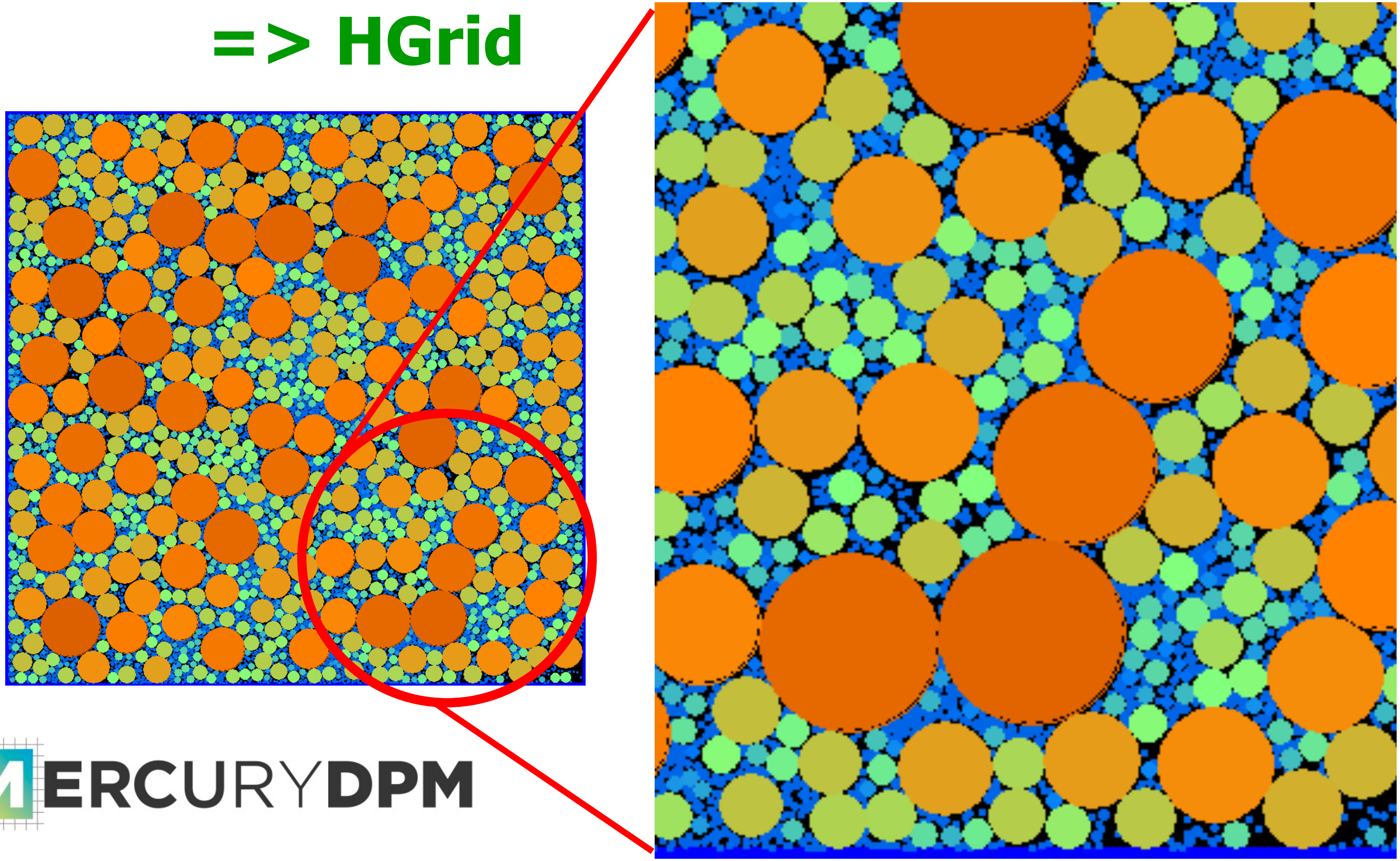


Example: Mixing



A. Gupta et al., MSM, 2010

Challenge: DEM with realistic sizes => HGrid



A. Ogarko et al., MSM, 2010-14

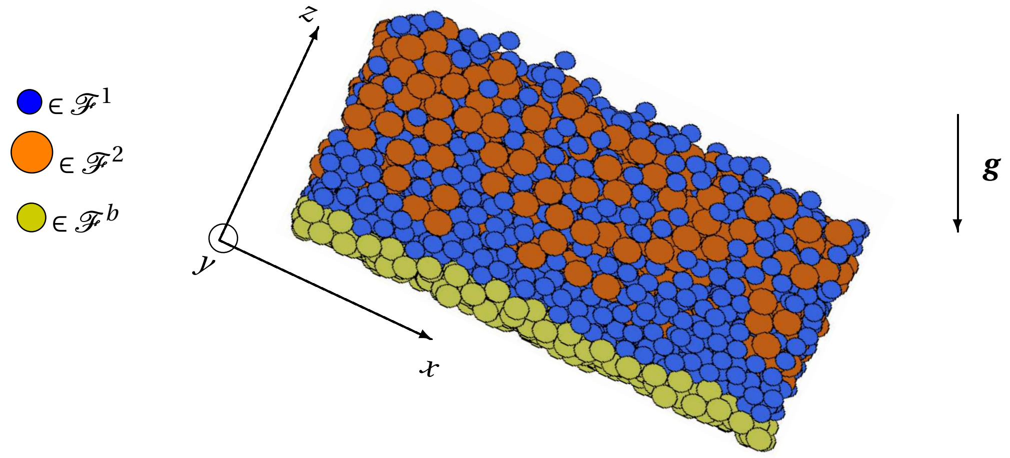
... highly polydisperse powders

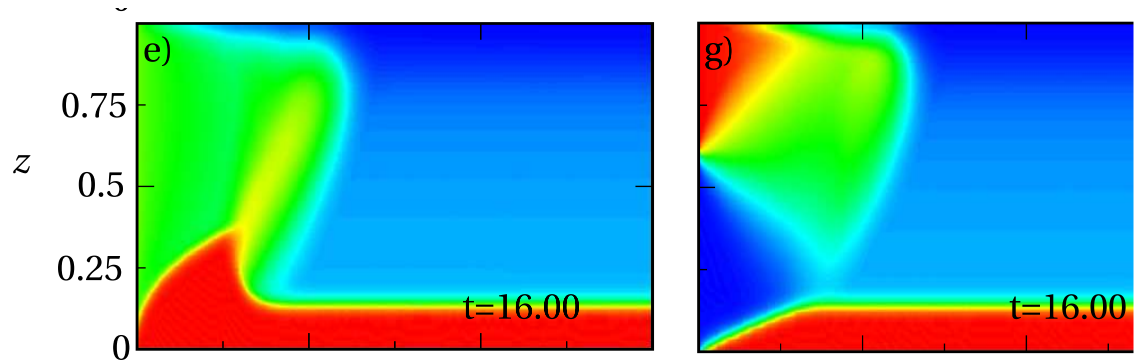
Shallow flow continuum equations (3D->2D)

D. Tunuguntla et al. 2016

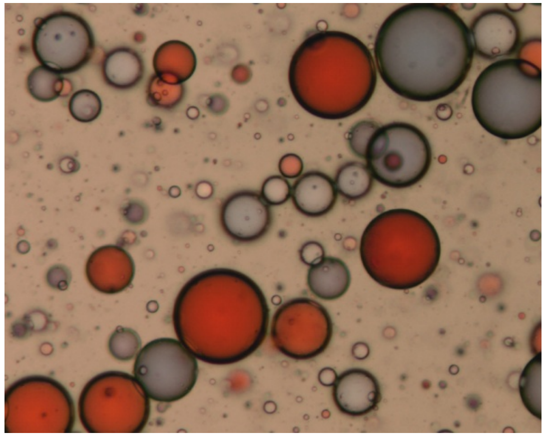
- D. Tunuguntla
  (PhD-thesis 2015)

- inspired & calibrated
  by experiment & DEM
- boundary conditions
- multi-species
  mixing & segregation
- erosion & sedim.





Different MATERIALs



FRICTIONLESS → **FRICTIONAL** → **COHESIVE**

F. Goncu, CRAS, 2010
O. I. Imole et al KONA, 2013
N. Kumar et al Particuology (2013)
N. Kumar et al. Acta Mechanica (2014), GM 2016

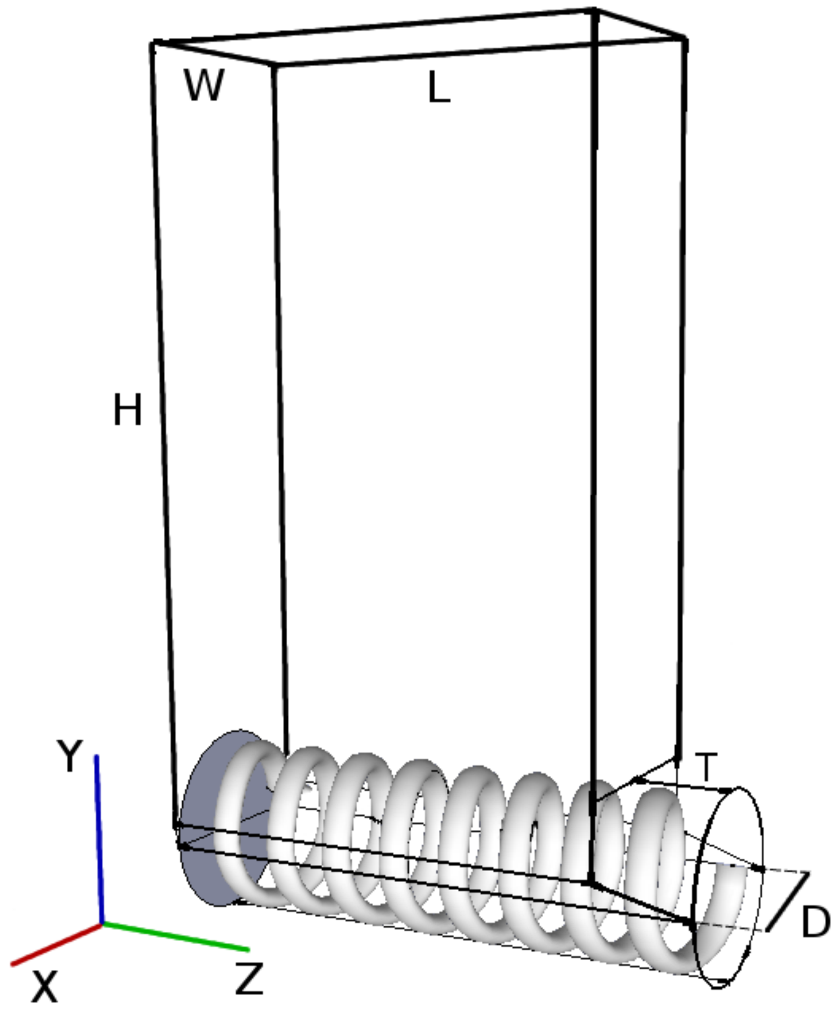
V. Magnanimo (2011-13)
O. I. Imole et al (2014-16)

S. Luding et al. (2001-13)
A. Singh et al. (2014-16)
S. Roy et al. (2015-17)

Pictures: J. Brujic et al. Nature 460 (2009)
Dijksman, Brodu, Behringer (2013-14)

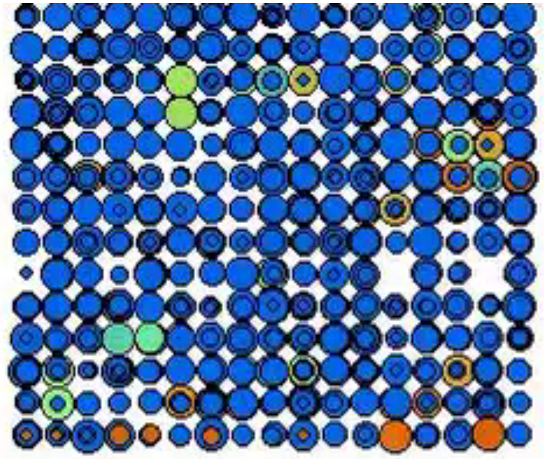
Open source

Based on:
- HGrid
- MicroMacro



Dosing application example …

MERCURYDPM



Open source

Based on:
- HGrid
- MicroMacro

flowable powder

(screw hidden)

© Marco Ramaioli, Nestle

Dosing application example …

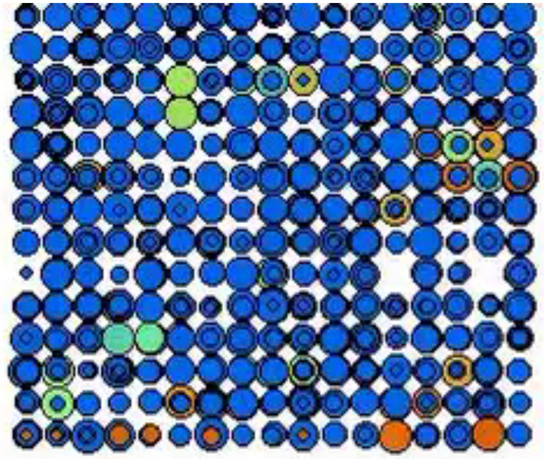
![MercuryDPM logo]

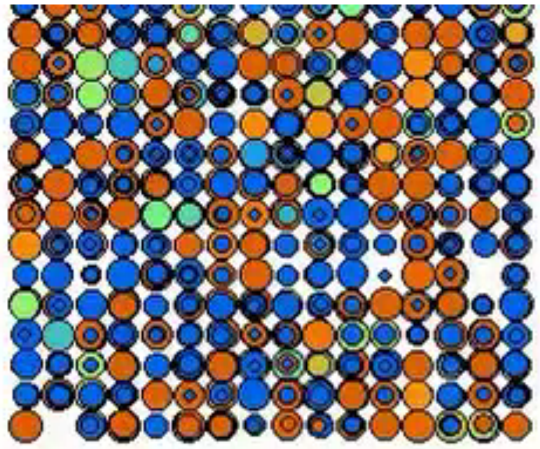
Open source

Based on:
- HGrid
- MicroMacro

flowable powder vs.
sticky, chunky powder

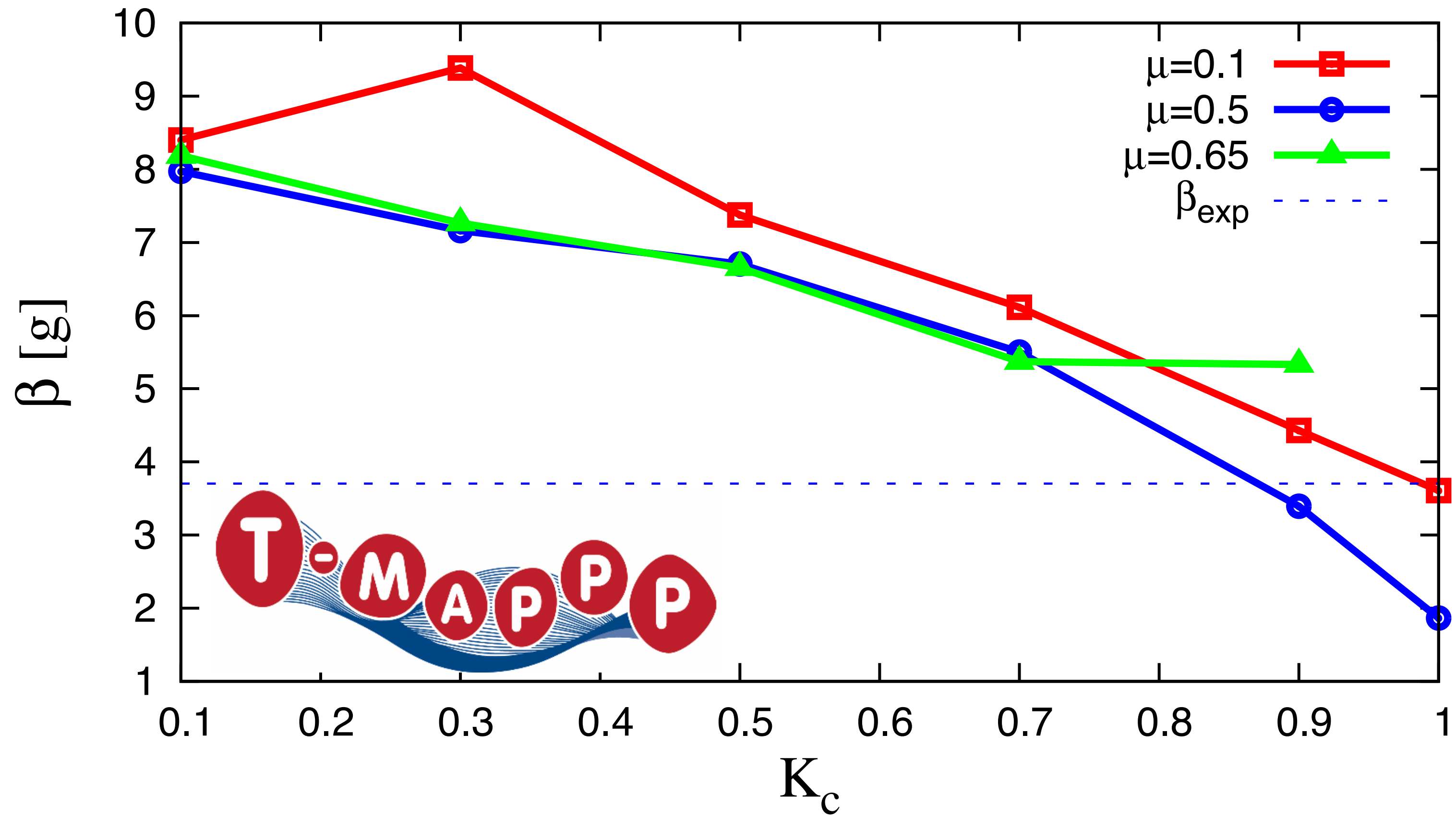
(screw hidden)





Dosing application example …

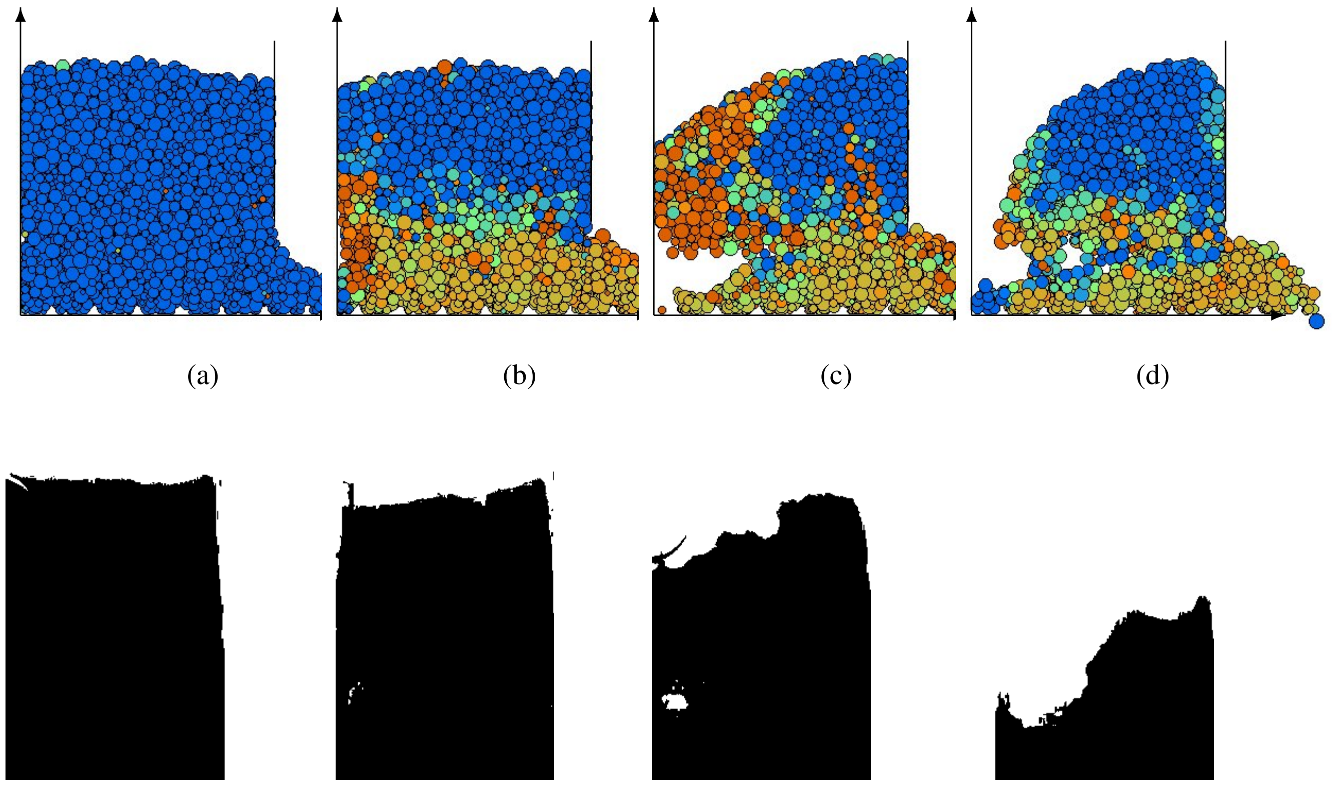
Dosing – parameter calibration



*Based on O. I. Imole, D. Krijgsman, T. Weinhart, V. Magnanimo, E. C. Montes, M. Ramaioli, and S. Luding, Powder Tech, 2016.

Experiments and Discrete Element Simulation of the Dosing of Cohesive Powders in a Canister Geometry. In preparation, PhD-thesis, O. I. Imole 2014

Dosing meso-rheology:
DEM vs. experiment <= Validation



(a) (b) (c) (d)

(e) (f) (g) (h)

*Based on O. I. Imole, D. Krijgsman, T. Weinhart, V. Magnanimo, E. C. Montes, M. Ramaioli, and S. Luding, Powder Tech, 2016.

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Software used …

- DEMSolutions/EDEM
- DCS/LIGGGHTS
- YADE
- **MercuryDPM**
- and some others …

Software used …

- DEMSolutions/EDEM
- DCS/LIGGGHTS
- YADE
- **MercuryDPM**
- and some others

unique features:
- open-source (really)
- parallel (tested >400 processors)
- HGrid for largely different particle sizes
- mercuryCG for coarse-graining to continuum
- analytical complex geometry-support

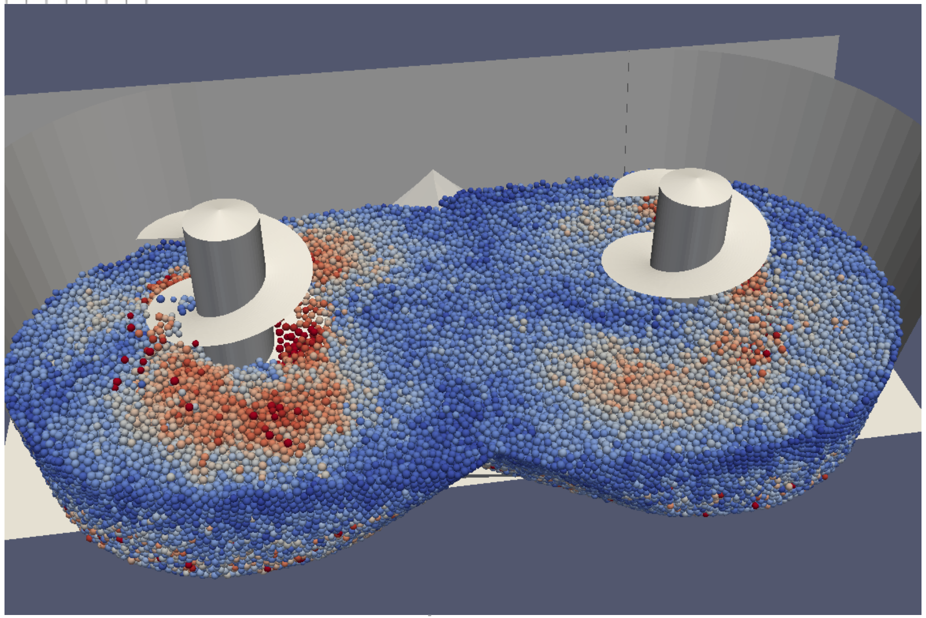
Software used …

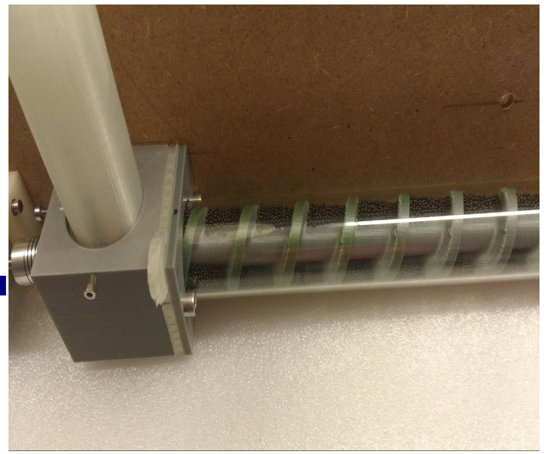
MERCURYDPM

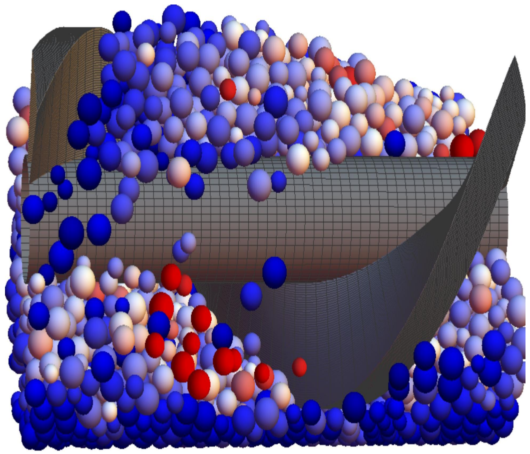
MercuryLab

- Mercury*Cloud* no need to buy hardware/pay on demand
- Training
- Expertise
- Support

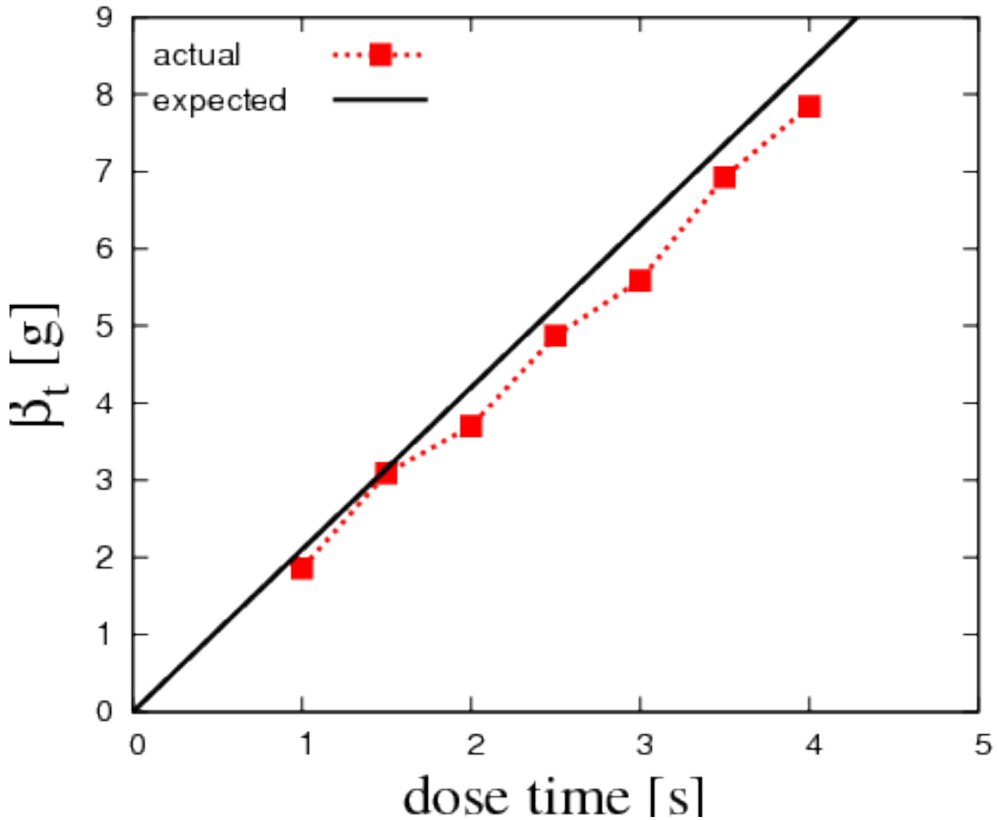
Realistic industrial designs (bad->good)







Dosing: DEM vs. experiment



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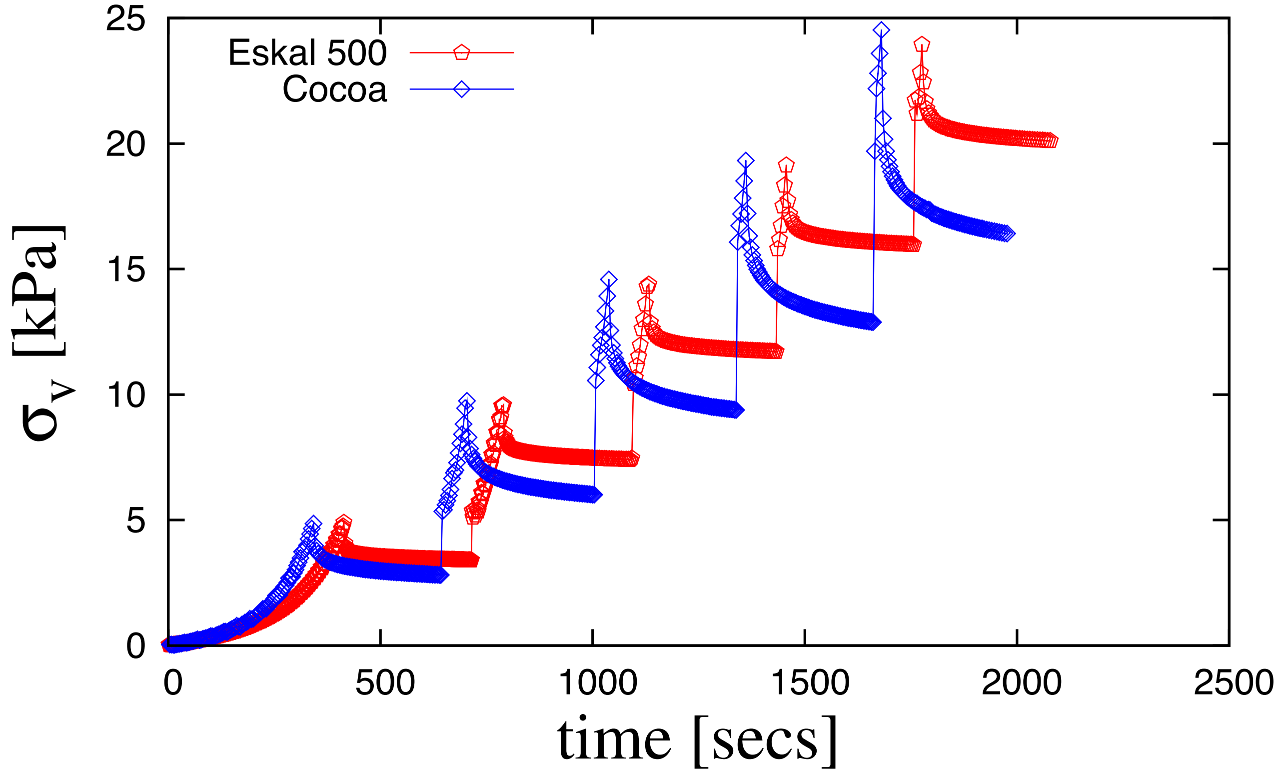
Experiments and Discrete Element Simulation of the Dosing of
Cohesive Powders in a Canister Geometry. In preparation, PhD-thesis, O. I. Imole 2014

Compaction & Creep: experiment – no DEM (yet)



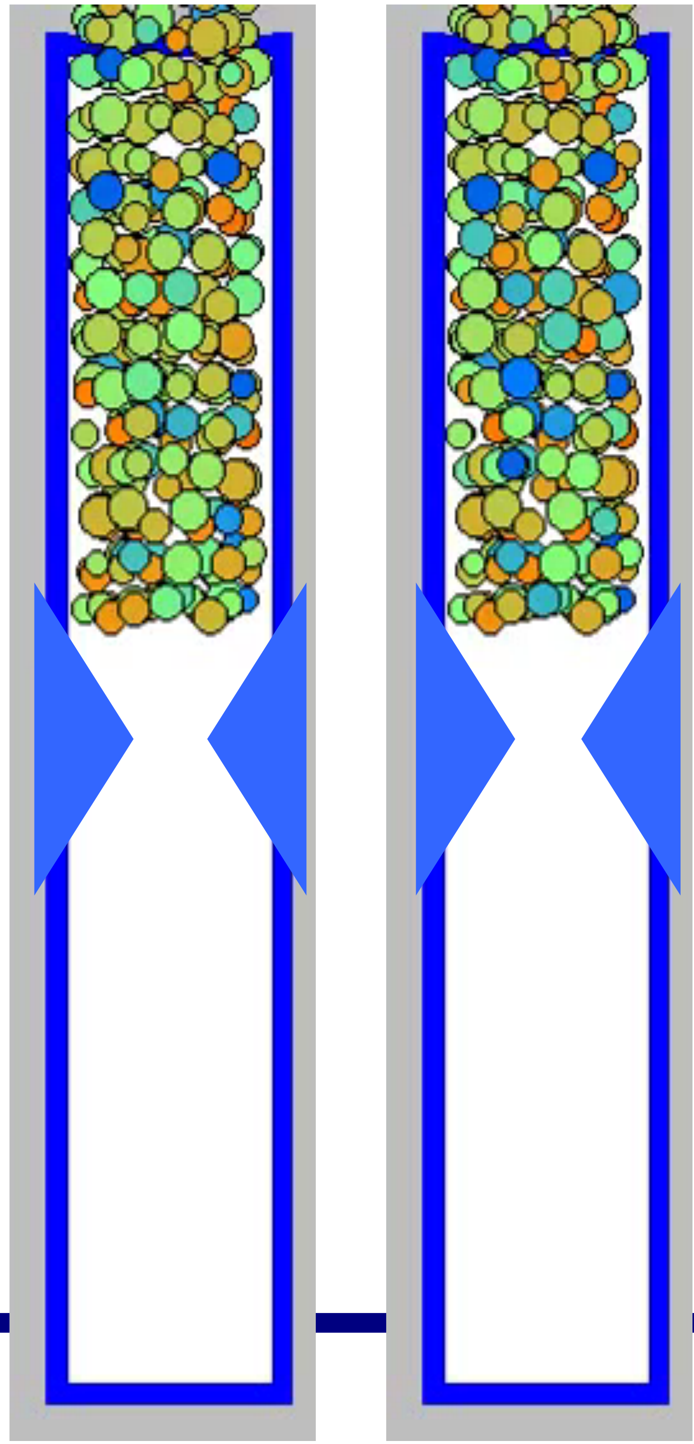
*Based on O. I. Imole, M. Paulick, M. Morgeneyer, V. Magnanimo, E. C. Montes, M. Ramaioli, A. Kwade, and S. Luding.

An experimental and theoretical investigation of the time-dependent relaxation behavior of cohesive powders, PhD-thesis, O. I. Imole, 2014-2016

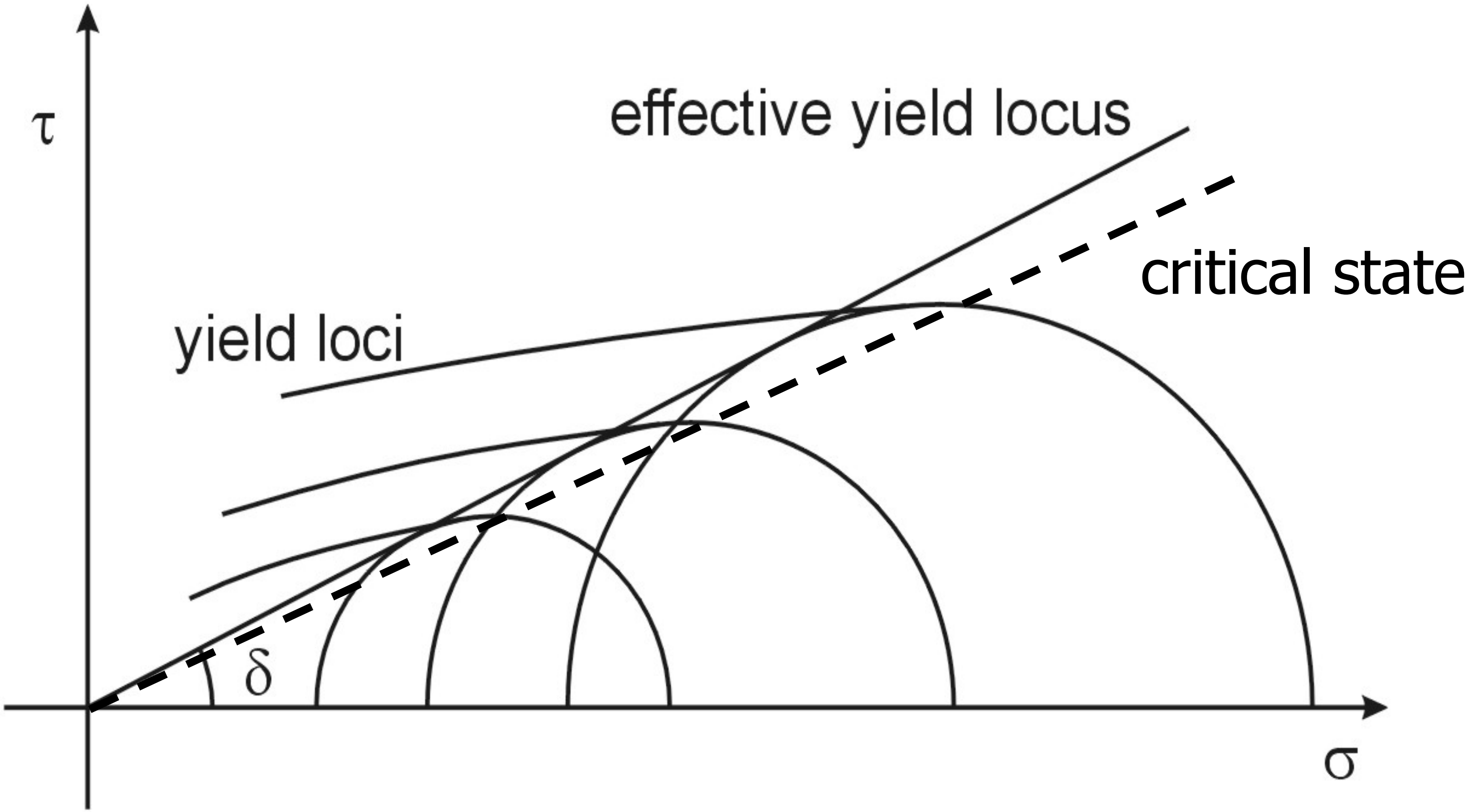
Particle systems

sometimes FLUID
sometimes SOLID
sometimes BOTH

un-jamming:
fluid <==> solid



Static: yield loci => steady state flow



Temporal-spatial coarse graining
discrete => continuum

- Define the macro-density using a coarse-graining function:

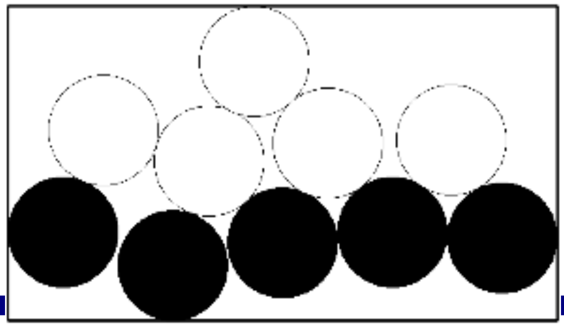
$$\rho(\mathbf{r}) = \sum_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}} \mathbf{m_i}\varphi(\mathbf{r} - \mathbf{r_i})$$

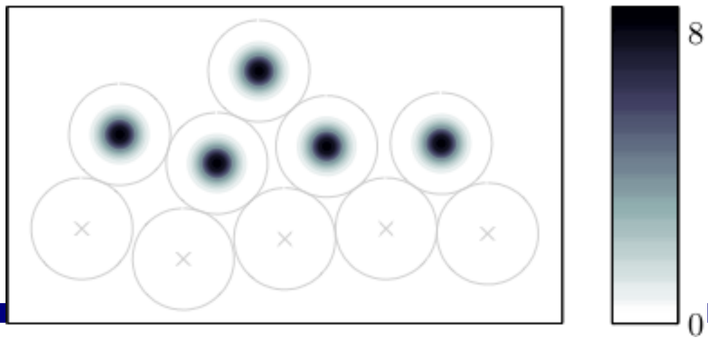
- Define velocity such that mass balance, $\partial\rho/\partial t + \nabla \cdot (\rho V) = 0$, is satisfied:

$$\mathbf{V} = \mathbf{p}/\rho, \text{ where } \mathbf{p} = \sum_{i=1}^{N} m_i \mathbf{v}_i \varphi(\mathbf{r} - \mathbf{r}_i)$$

- weight function:

$$\varphi(\mathbf{r}) = \frac{1}{(\sqrt{2\pi}w)^3}\exp\left(-\frac{|\mathbf{r} - \mathbf{r}_i|^2}{2w^2}\right)$$



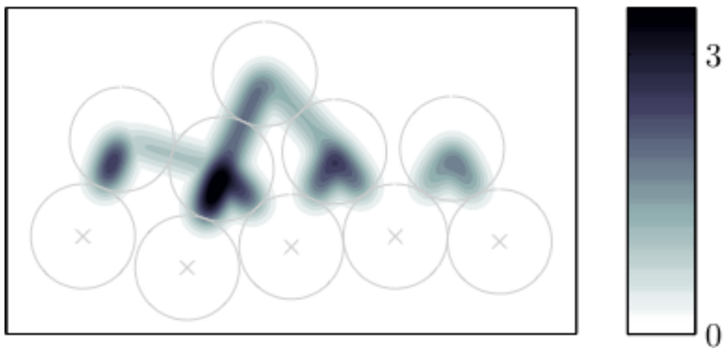


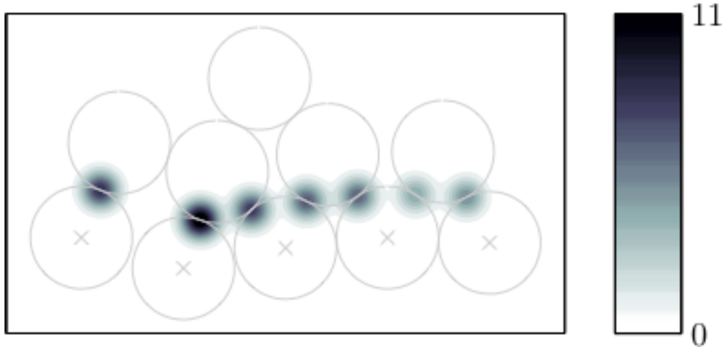
Density ρ for a 2D-Gaussian coarse-graining function.
w = d/8.

Temporal-spatial coarse graining
discrete => continuum

- Define stress and wall drag
  such that momentum balance is satisfied

$$
\begin{aligned}
\boldsymbol{\sigma}^k &= -\sum_{i=1}^N m_i \mathbf{v}_i' \mathbf{v}_i' \varphi(\mathbf{r}-\mathbf{r}_i) \\
\boldsymbol{\sigma}^c &= -\sum_{c_{ij}} \mathbf{f}_{ij}\mathbf{r}_{ij} \int_0^1 \varphi(\mathbf{r}-(\mathbf{r}_i + s\mathbf{r}_{ij}))ds \\
&\quad -\sum_{w_{ik}} \mathbf{f}_{ik}\mathbf{a}_{ik} \int_0^1 \varphi(\mathbf{r}-(\mathbf{r}_i + s\mathbf{a}_{ij}))ds \\
\mathbf{t} &= -\sum_{w_{ik}} \mathbf{f}_{ik}\varphi(\mathbf{r}-\mathbf{c}_{ik})
\end{aligned}
$$



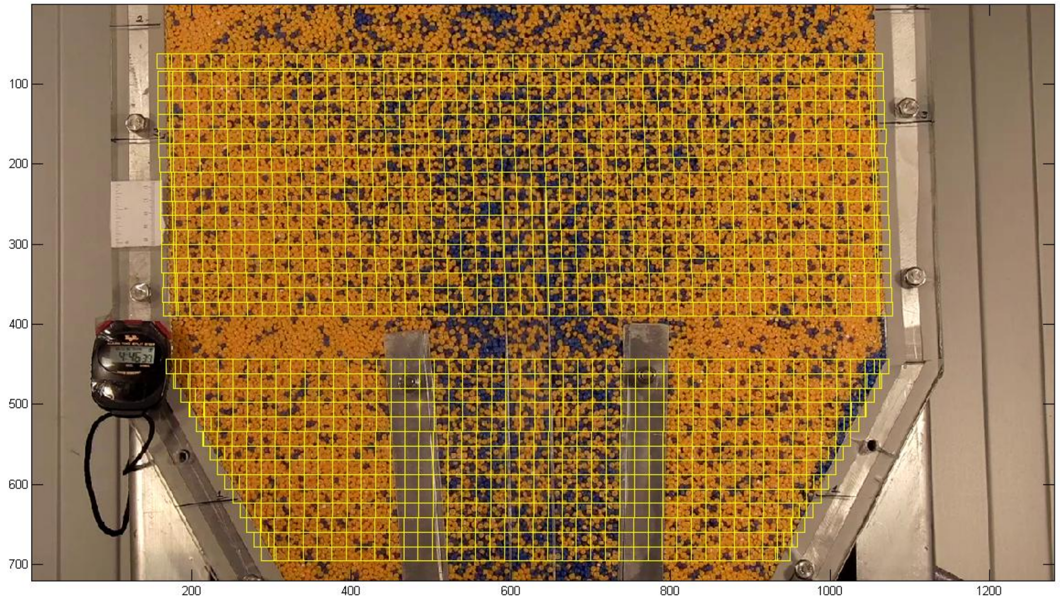


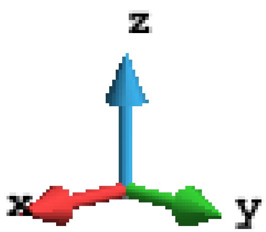
Weinhart, T., Thornton, A.R., Luding, S., Bokhove, O., From discrete particles to continuum fields near a boundary. Granular Matter 14(2), 289-294 (2012)

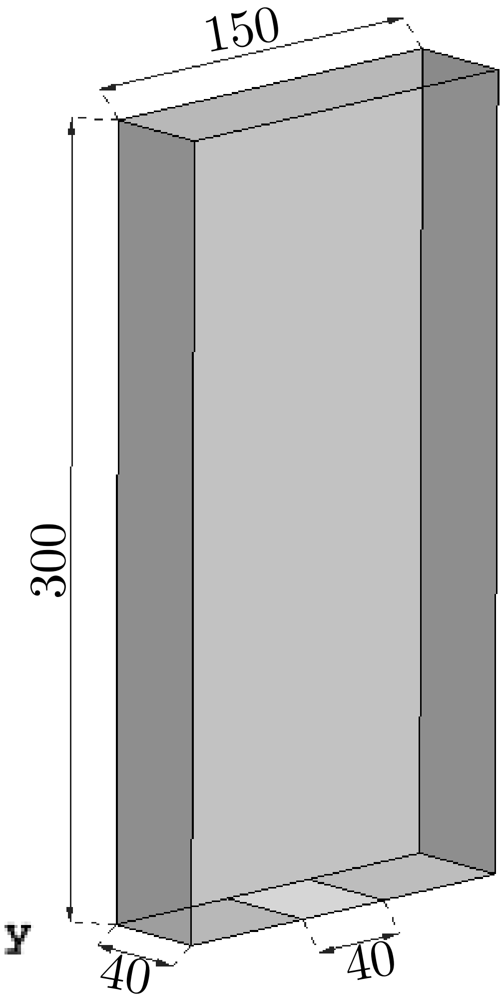
Test case: Silo flow model

Silo flow model with internal flow pattern is used

- *Stagnant zone – core flow*
- *High shear-rate localization zone*
- *Fast core flow zone*



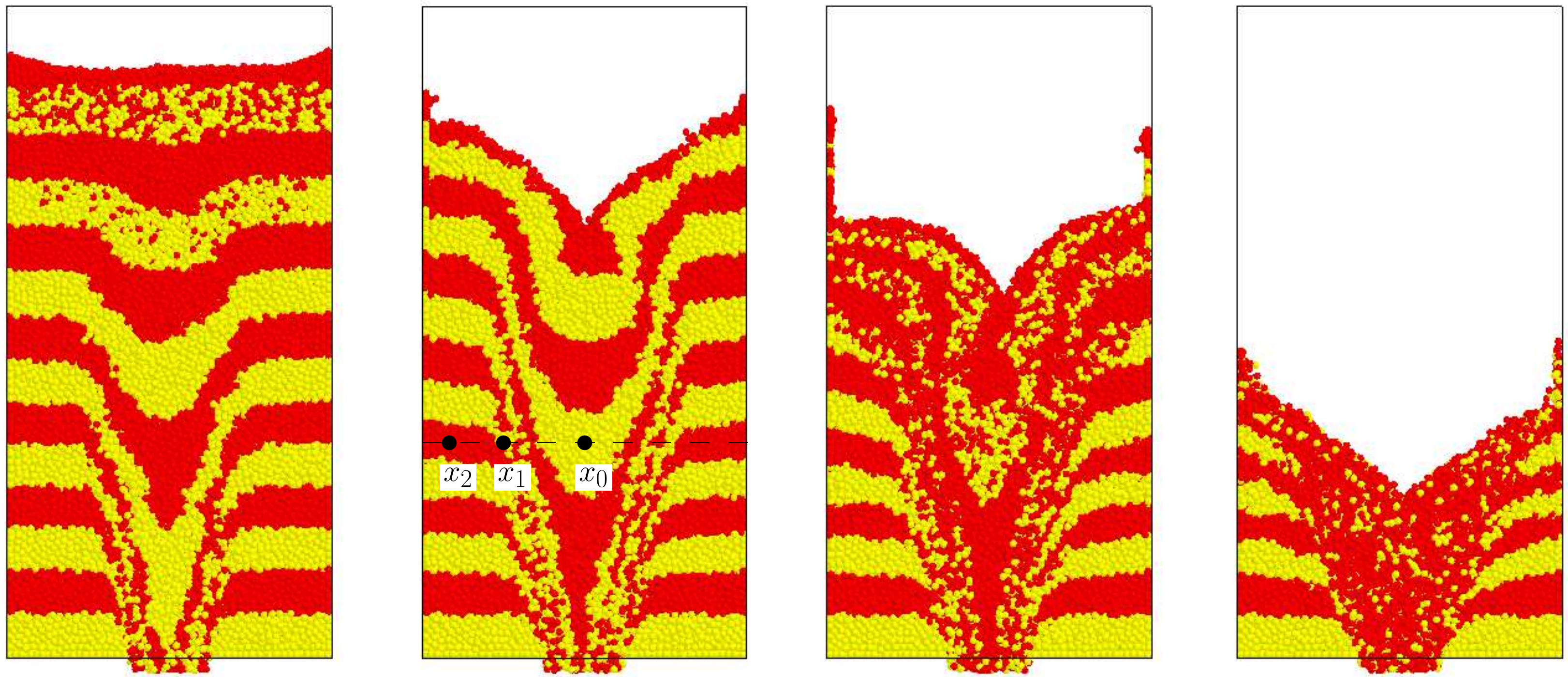




- Experiments: UEdinburgh

Test case: Silo flow model

Silo flow model with internal flow pattern is used

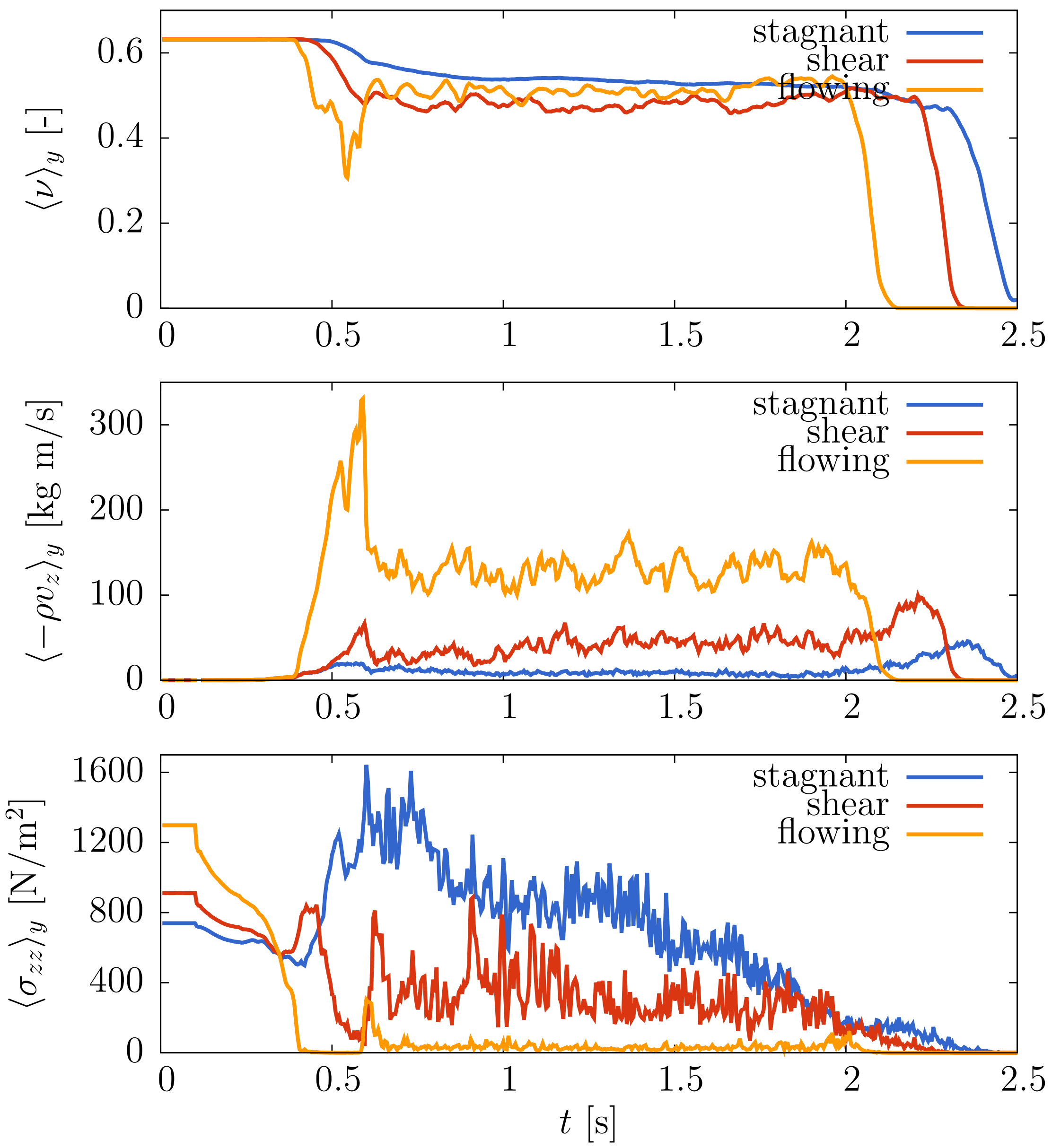


(a) t=0.745s (b) t=1.200s (c) t=1.490s (d) t=2.240s

T. Weinhart et al., Powder Tech., 2016

Test case: Silo flow model

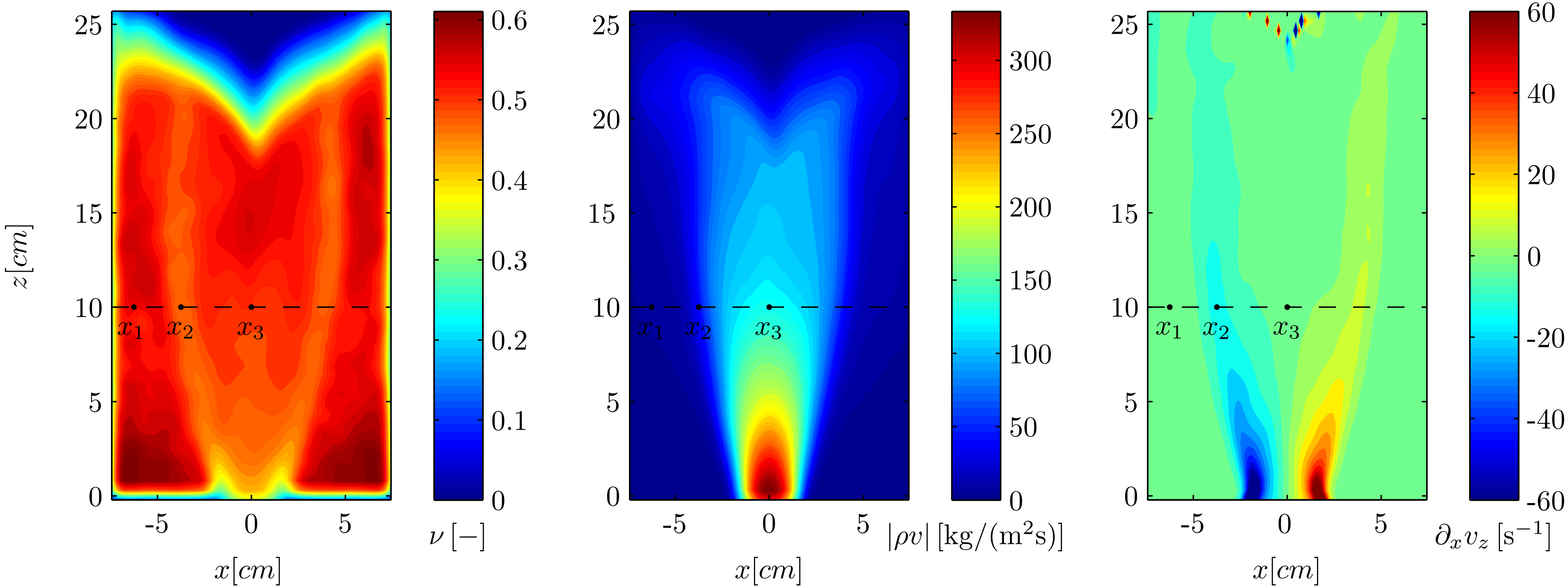
Horizontal variation:



T. Weinhart et al., Powder Tech., 2016

Test case: Silo flow model

Horizontal variation – different fields:



T. Weinhart et al., Powder Tech., 2016

shear band – which field?

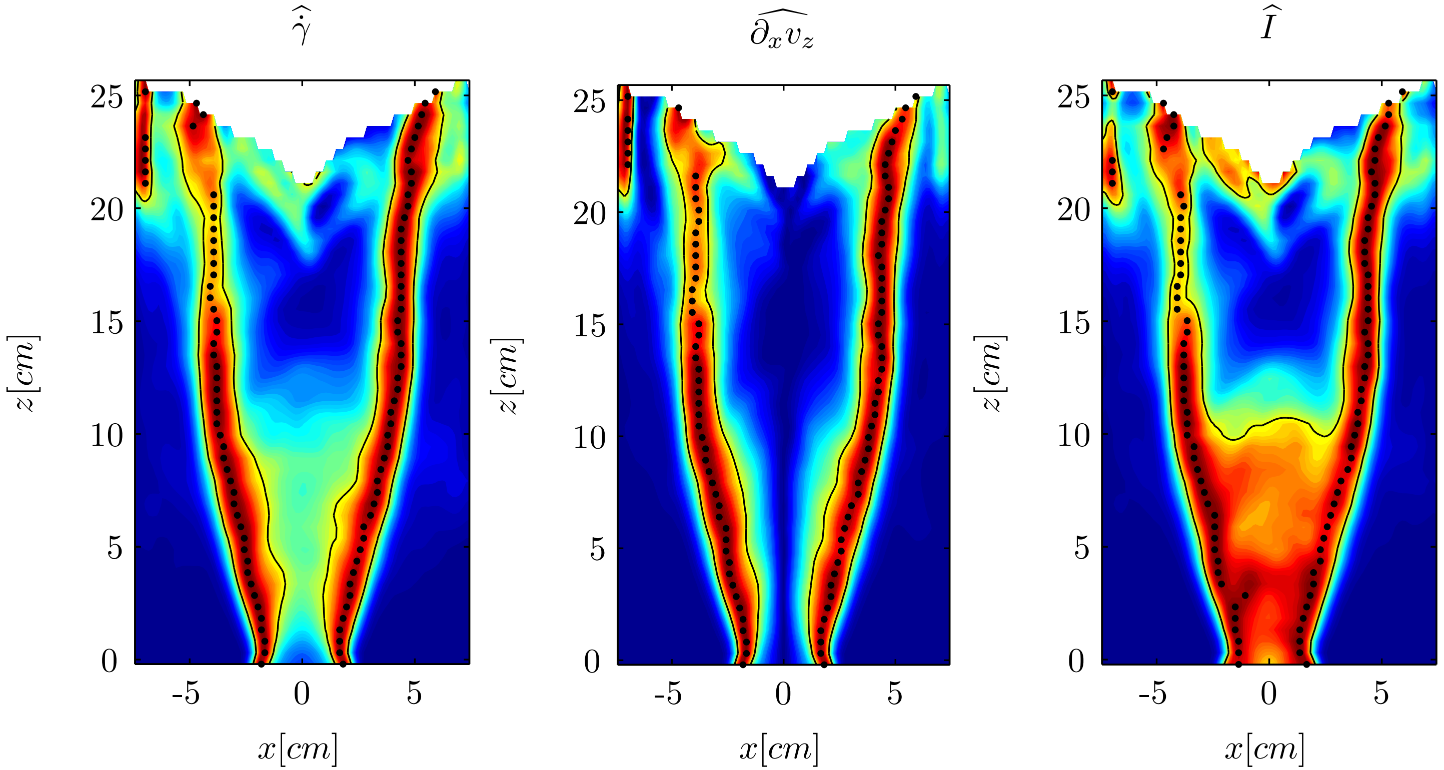
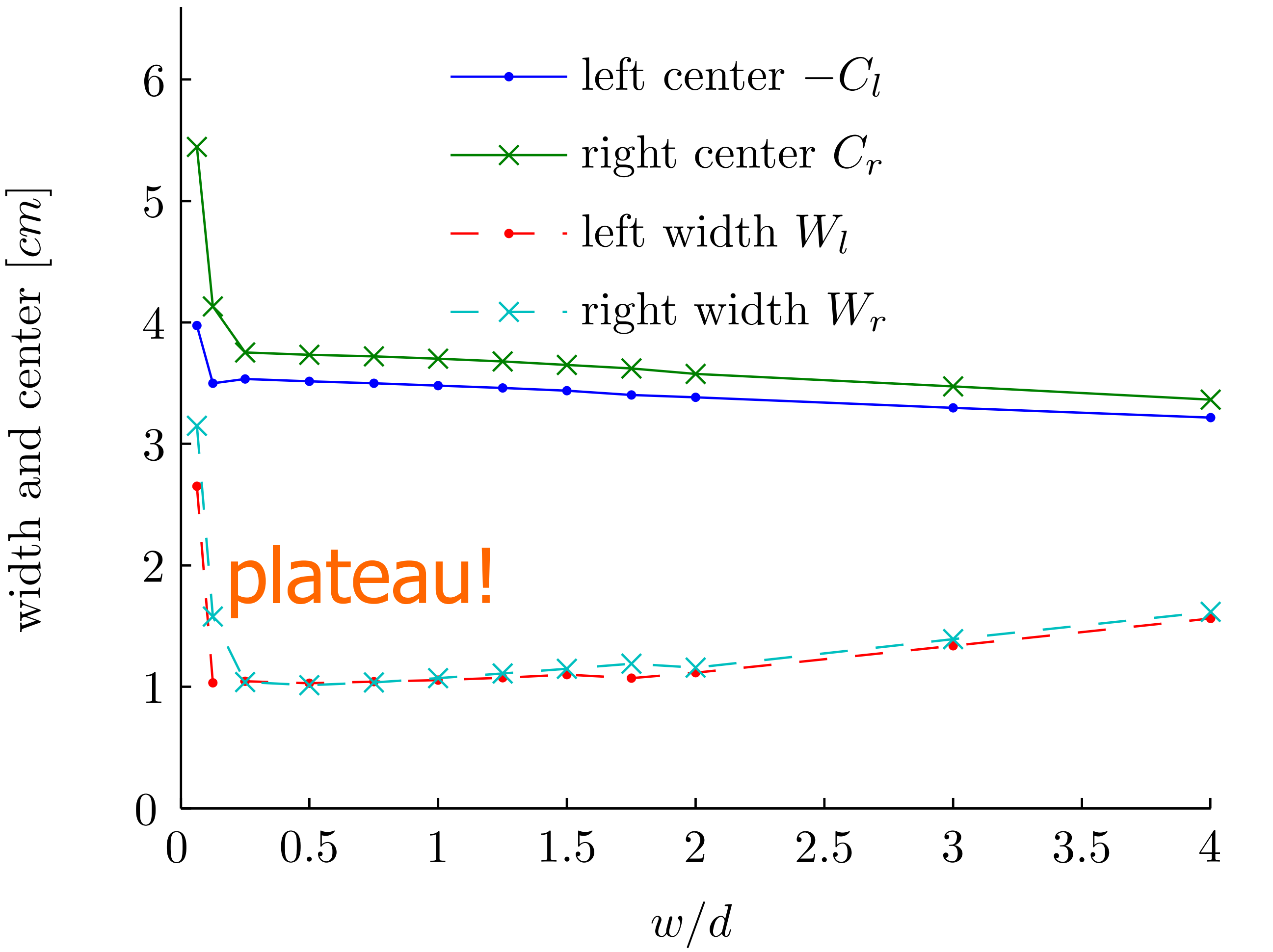


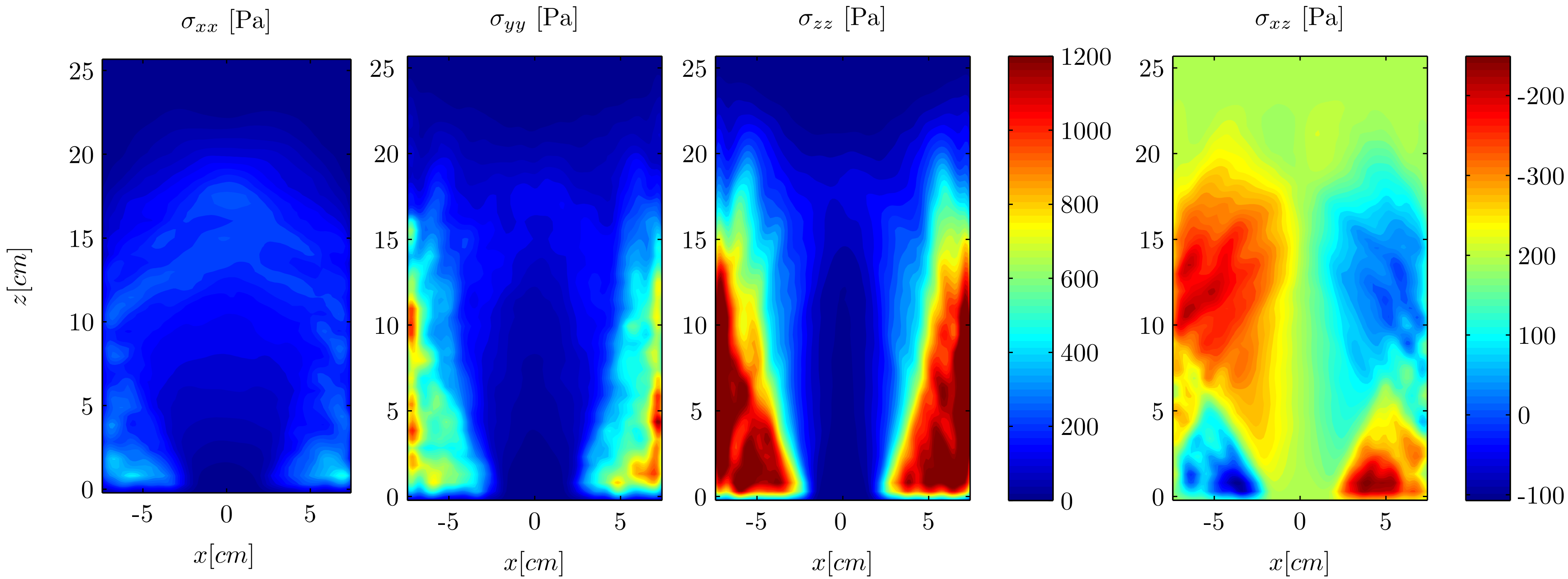
Figure 12: Tensorial shear rate $\dot{\gamma}$, horizontal shear rate $\partial_x v_z$, and inertial number $I = \frac{\dot{\gamma} d}{\sqrt{p/\rho_p}}$ scaled onto the interval $[0, 1]$ by its maximum at each height, see (16). Data for $\nu < 0.1$ (white area on the top) is not considered. Dots denote the maxima of the depicted values in the left and right half of the domain, black contours denote demarcation of the shear band where the scaled value is less than a tolerance ($tol = 0.6$). All values averaged over y and $1 \leq t \leq 1.4$ for $w = d$.

T. Weinhart et al., Powder Tech., 2016

shear band – which w (CG-width)?



stress components



T. Weinhart et al., Powder Tech., 2016

Discrete to continuum
Micro-macro: coarse-graining

- micro-macro CG applied to silo flow example
- Influence of CG parameters analysed

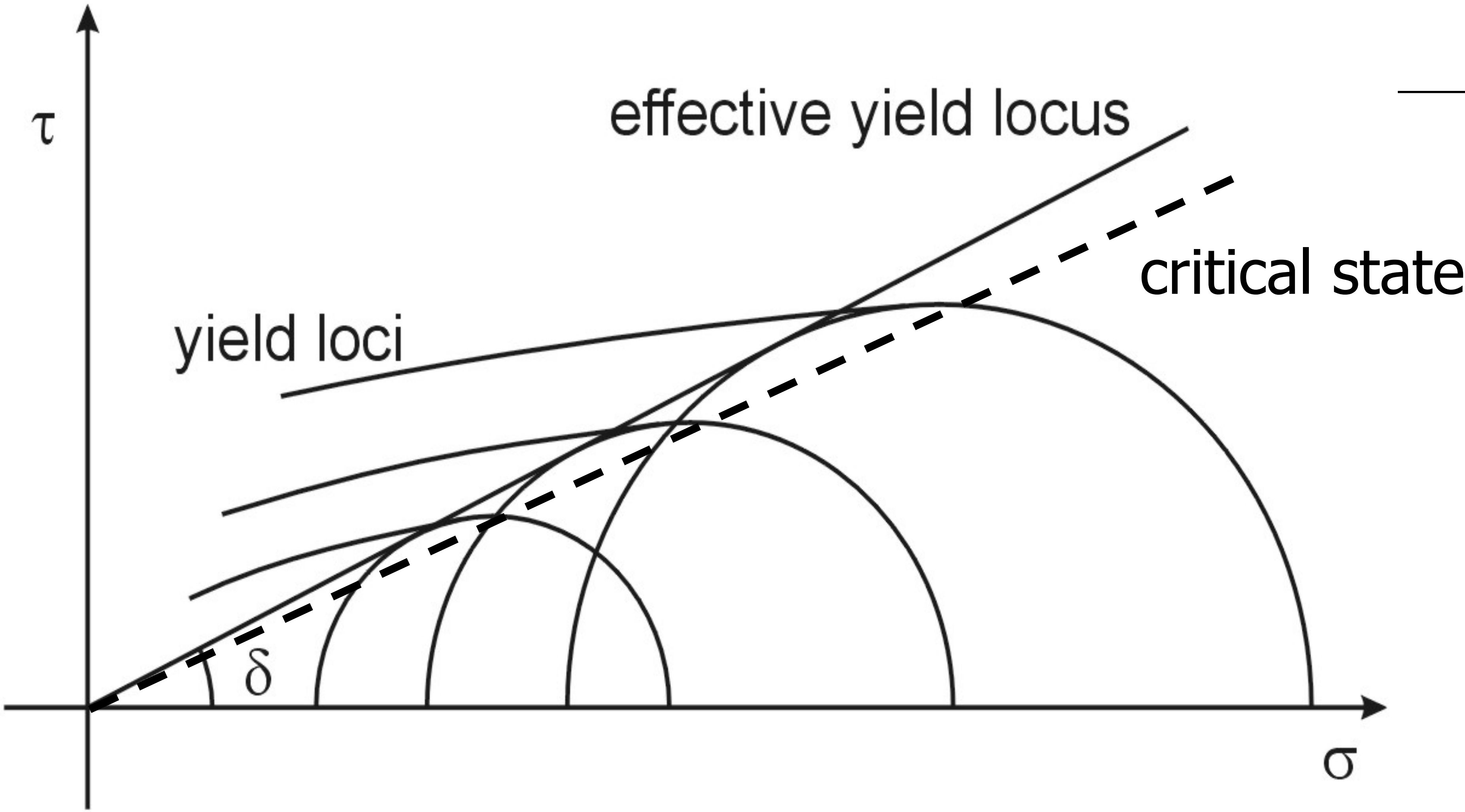
  Macro-variables should be independent of both
  temporal and spatial averaging scale.

- Study of shear bands
- Study of bulk and wall stress

  - Anisotropic normal bulk stresses with signs of force chains & arches

- Next? use those results from DEM for your purpose!
- From academic research to **industrial application**!

Static: yield loci => steady state flow



Introduction

• Granular materials are the combination of **discrete** solid (macroscopic) particles

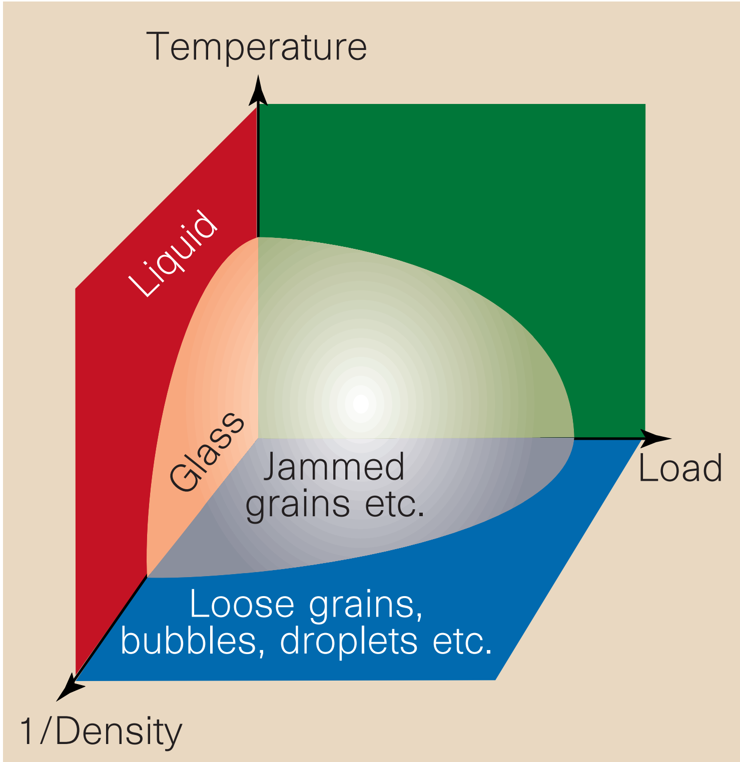
• **many interesting phenomena - can we understand them? all together?**

history-dependence, slow relaxation, creep/aging, shear-localization, “avalanches”, …

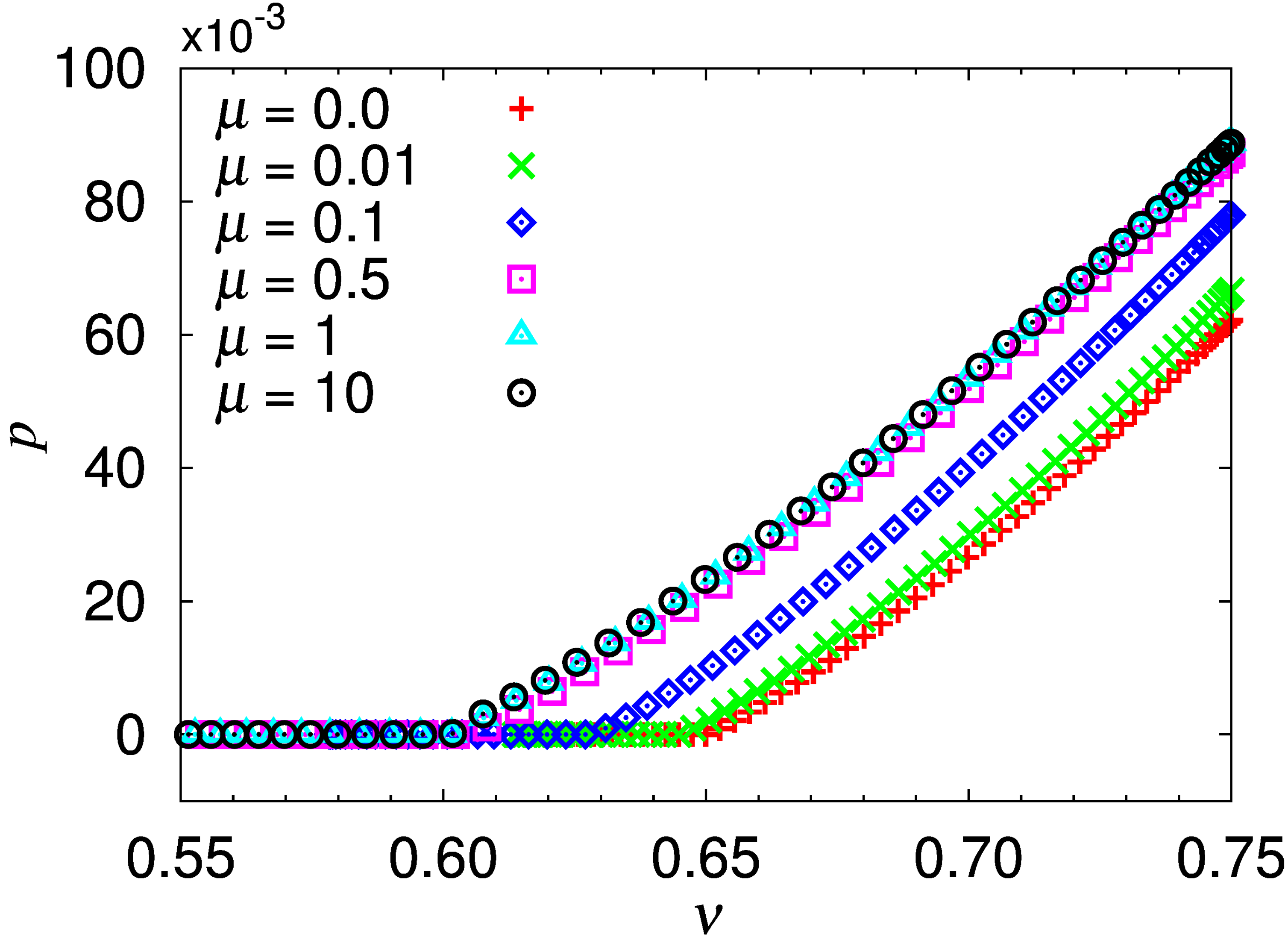
fluid-solid transition => jamming “point”

A. Liu and S. Nagel, Nature 396, 1998

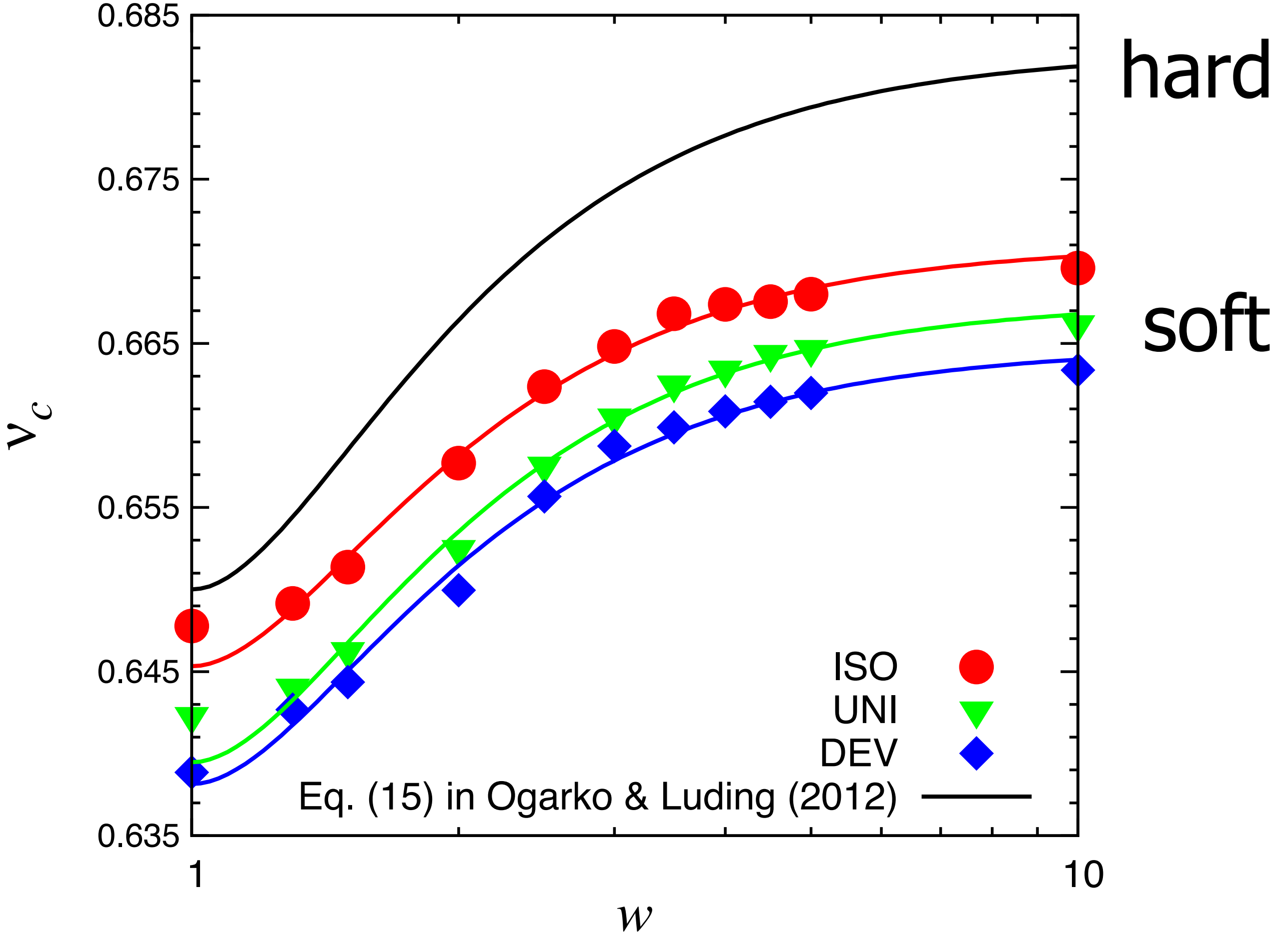
Examples:



Isotropic de-compression; effect of friction



Polydispersity and what's the difference between ISO, UNI and SHEAR?



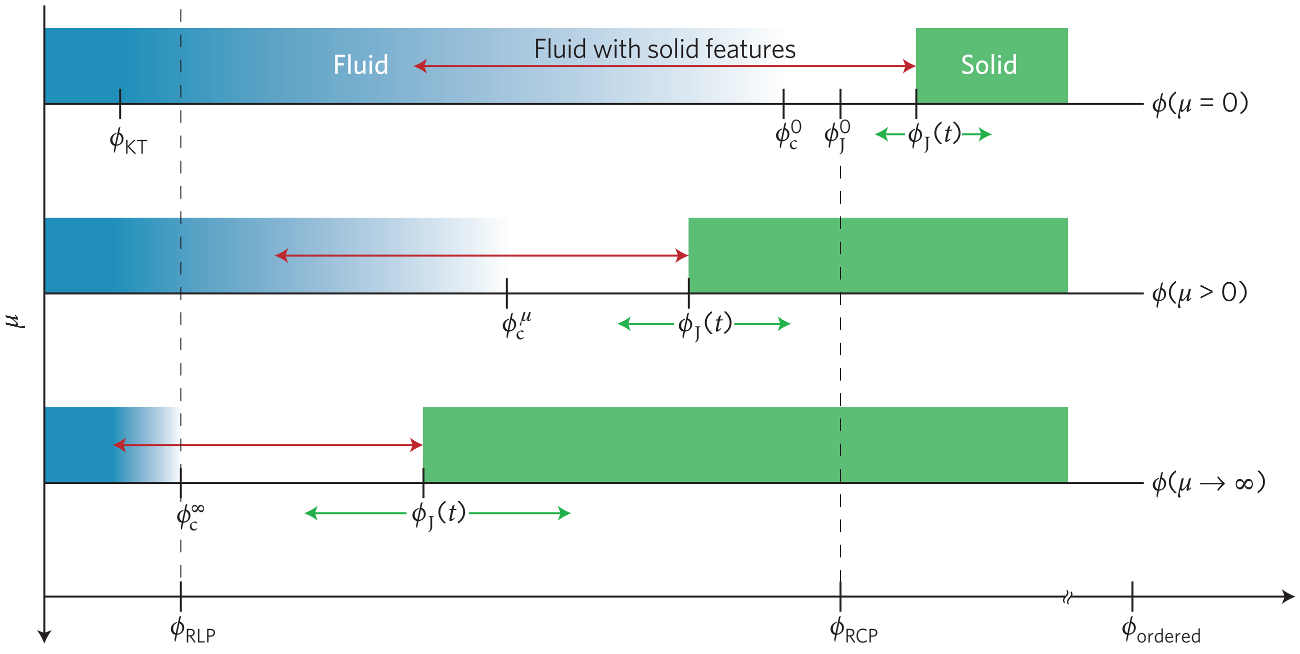
Jamming ⇔ unjamming (rheology)

• Granular materials are the combination of **discrete** solid (macroscopic) particles

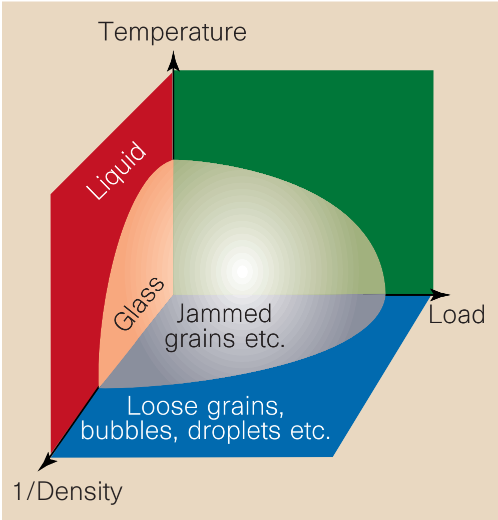
• **many interesting phenomena - can we understand them? all together?**

history-dependence, slow relaxation, creep/aging, shear-localization, “avalanches”, …

fluid-solid transition => jamming “~~point~~” – no point, but a variable! J-line!



S. Luding, Nature, 2016; Kumar, SL, GM, 2016



A. Liu and S. Nagel, Nature 396, 1998

Constitutive Model: With Anisotropy

Isotropy (before) + Anisotropy F_{dev}

$$
\begin{aligned}
\delta P^* &= 3B\delta\varepsilon_v + \boxed{A_1} S_\sigma \delta\varepsilon_{\rm dev}, \\
\delta\sigma^*_{\rm dev} &= 3\boxed{A_2}\delta\varepsilon_v + G^{\rm oct} S_\sigma \delta\varepsilon_{\rm dev}, \\
\delta F_{\rm dev} &= \beta_F \,{\rm sign}\left(\varepsilon_{\rm dev}\right) F^{\rm max}_{\rm dev} S_F \delta\varepsilon_{\rm dev}
\end{aligned}
$$

Due to $\boldsymbol{A_1}$ and $\boldsymbol{A_2}$, the model provides a **cross coupling** between the two types of stress and strain in the model

Need to define - Initial state and the deformation path

… then integrate the incremental evolution …

Constitutive model – calibration

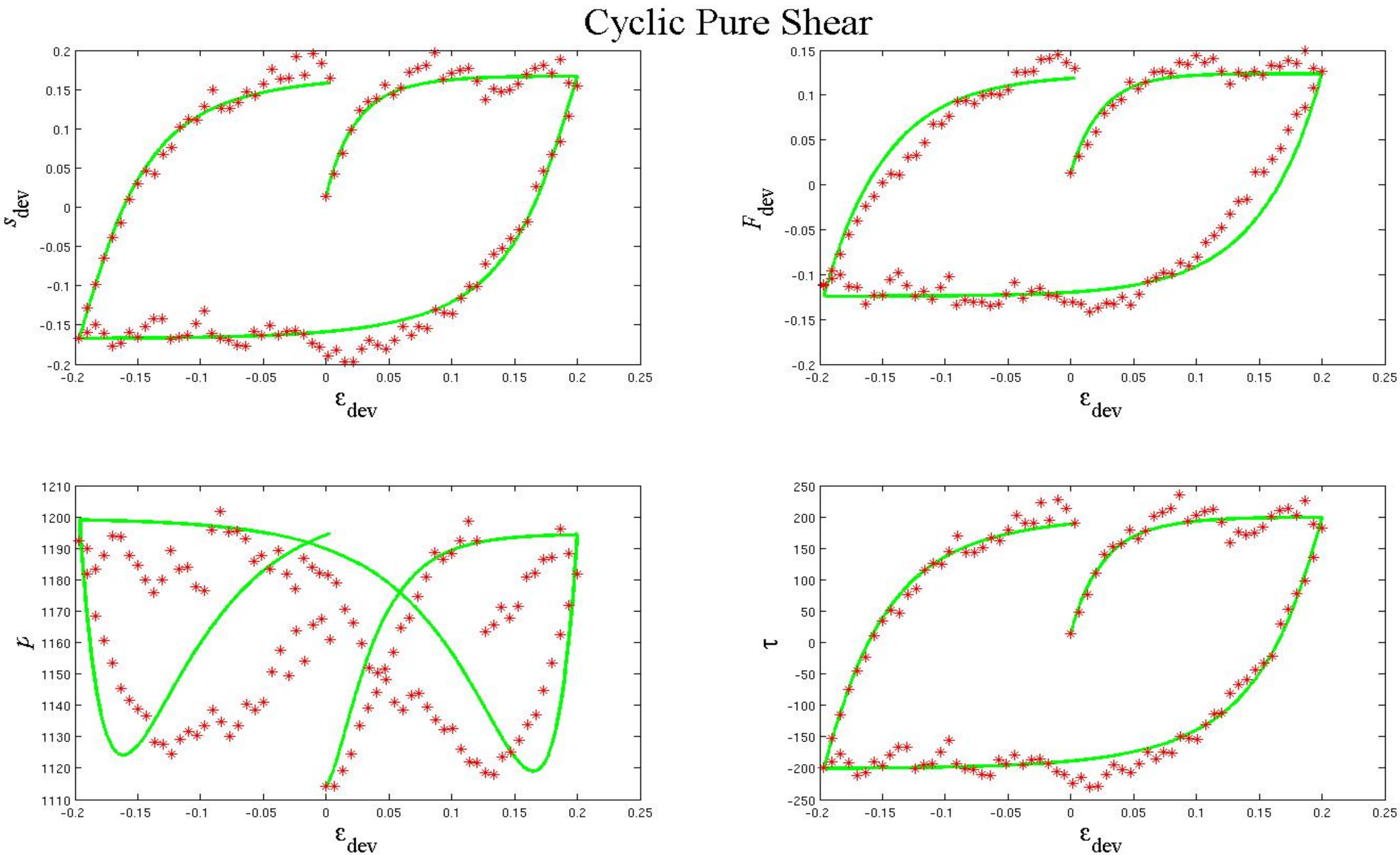
Direct moduli (B,G,A) probing …

Bulk Modulus: $B = b_0 F_V$

Shear Modulus: $G = B\, g(F_V)\, [1-\sigma^*_{dev} F_{dev}]$

Anisotropy Modulus: $A = B\, F_{dev}$

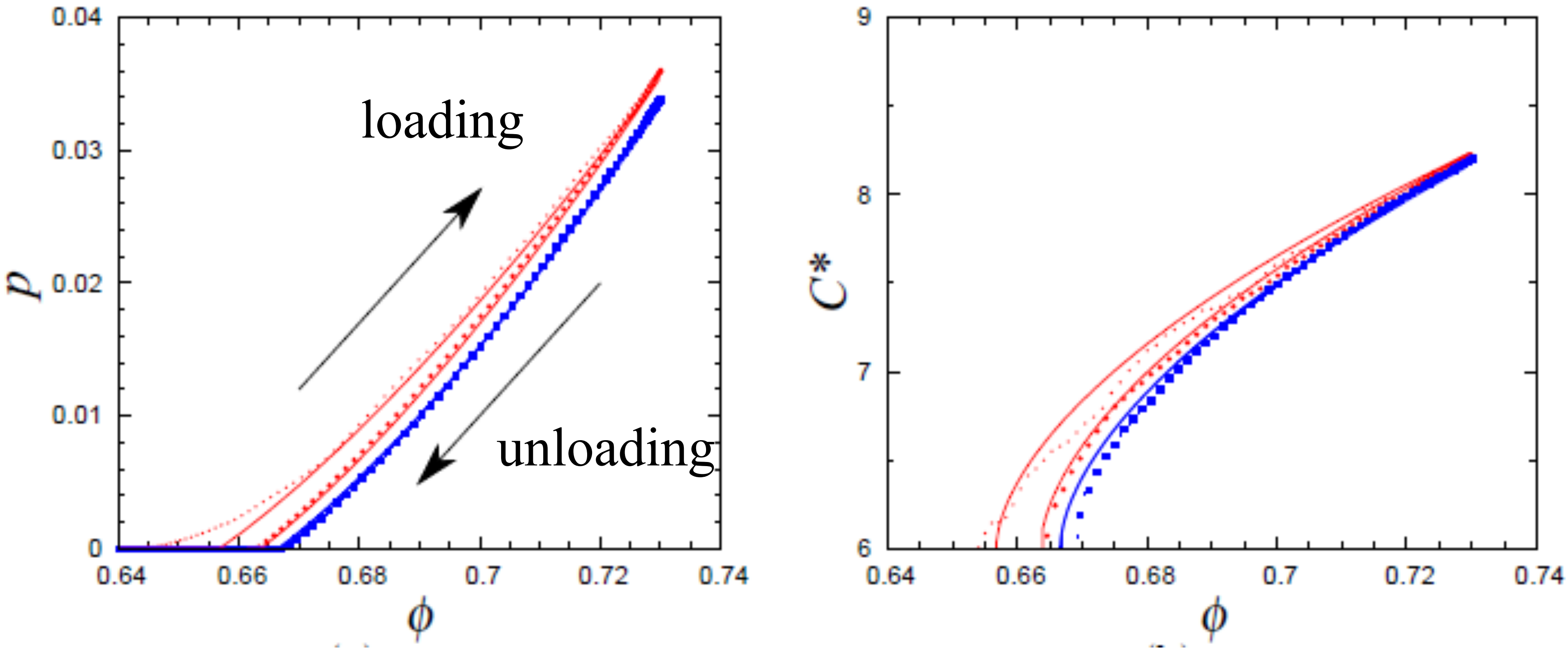
Prediction (improved 2014) – Cyclic Shear



N. Kumar, S. Luding, V. Magnanimo, Acta Mechanica, 2014

cyclic (isotropic) deformation

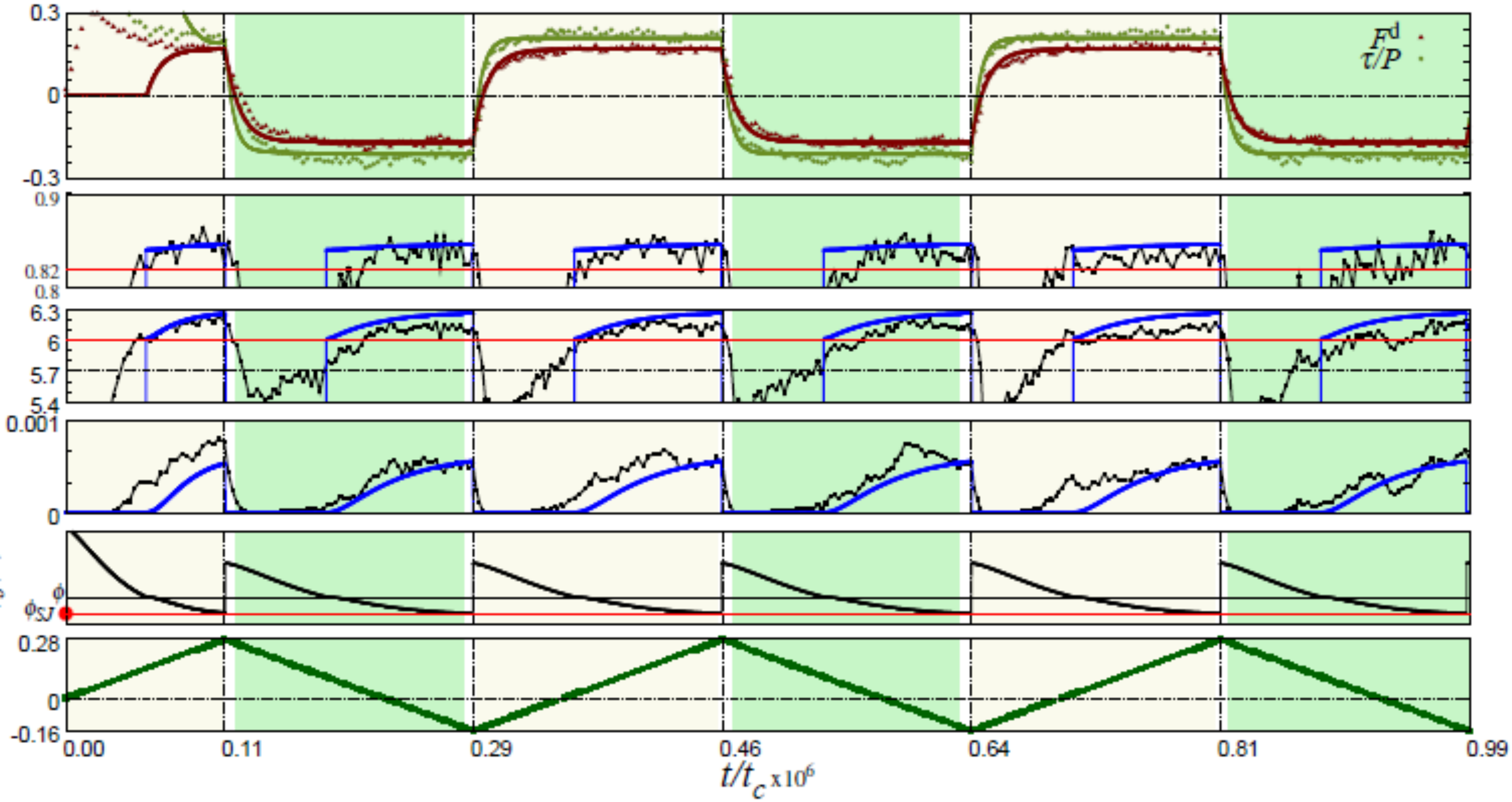
- Intermediate cyclic over-compression (amplitude 0.73)
- red: 1st cycle … blue: 100th cycle …



points: particle simulation ⇔ lines: continuum model (RVE)

Predictive power – cyclic pure shear MACRO

- Cyclic shear for 3 cycles (after the first loading, system forgets history).



- Quantities like – fraction of non-rattlers, coordination number, pressure – by mainly modifying the constitutive model with non-constant jamming point.

Summary:

there are isotropic & deviatoric modes of deformation!

- **dilatancy** in frictionless&frictional packings
- **elasticity** (reversible) plasticity (irreversible)
- *shear-jamming or thickening(?)* in frictionless packs
- **new** isotropic-state-variable! (for macro-view)

=> the jamming density $\Phi_J(H)$

... or another related quantity

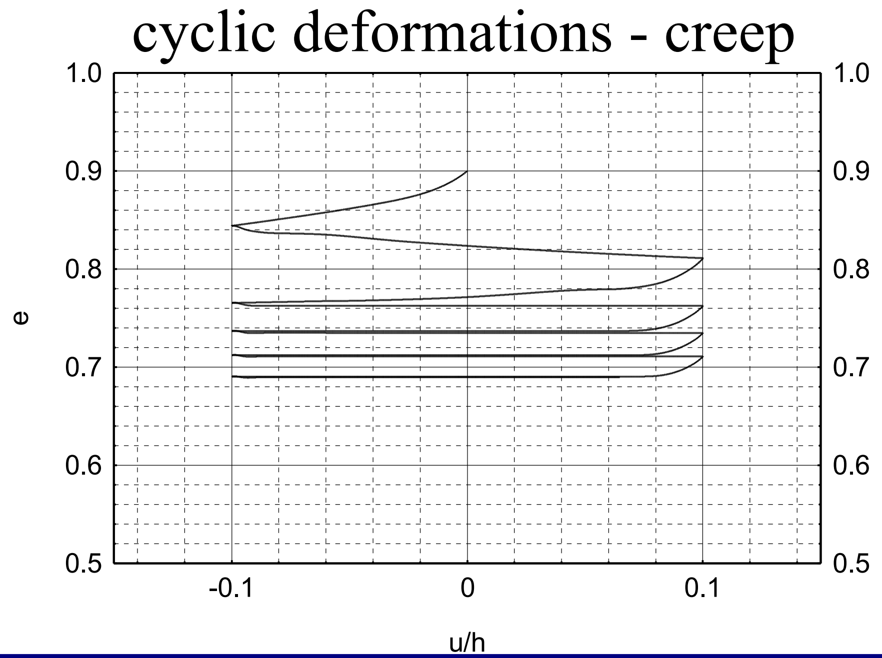
- fluctuations are missing => **meso-scale**
- energy-landscape model explains it all ☺

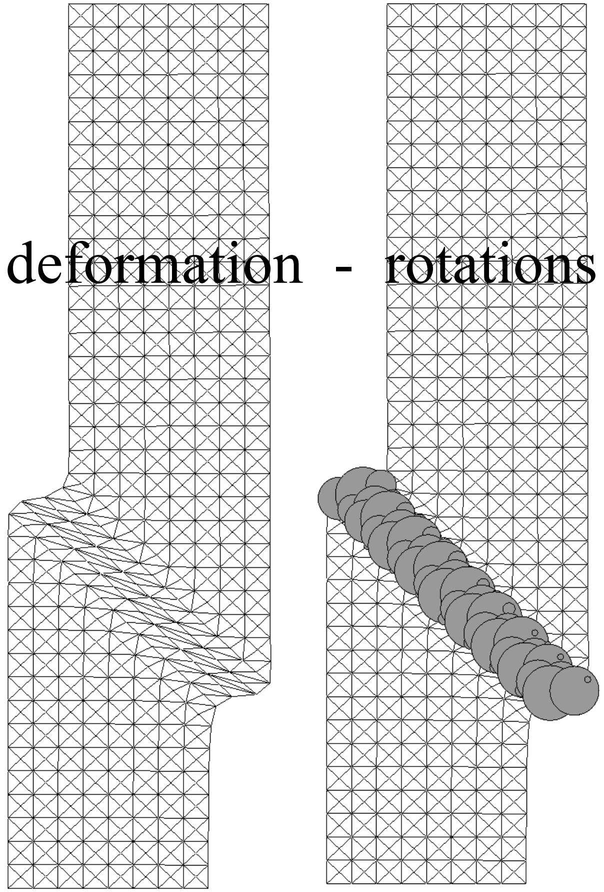
Next: Implementation in FEM model

+ successful tool – few parameters

- microscopic foundations ?

- extensions & parameter identification

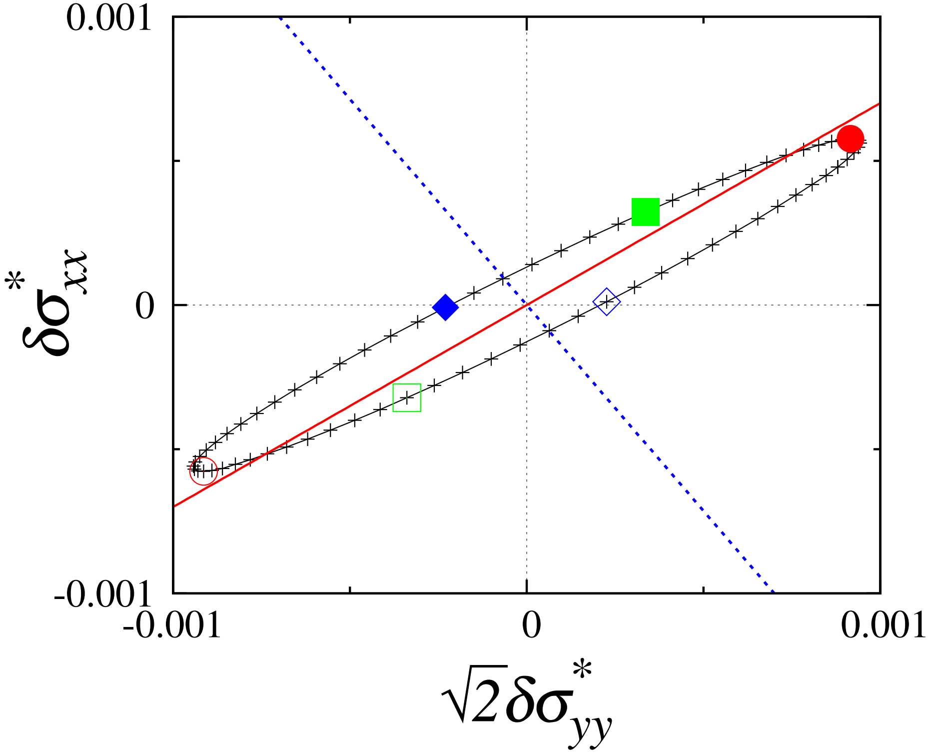


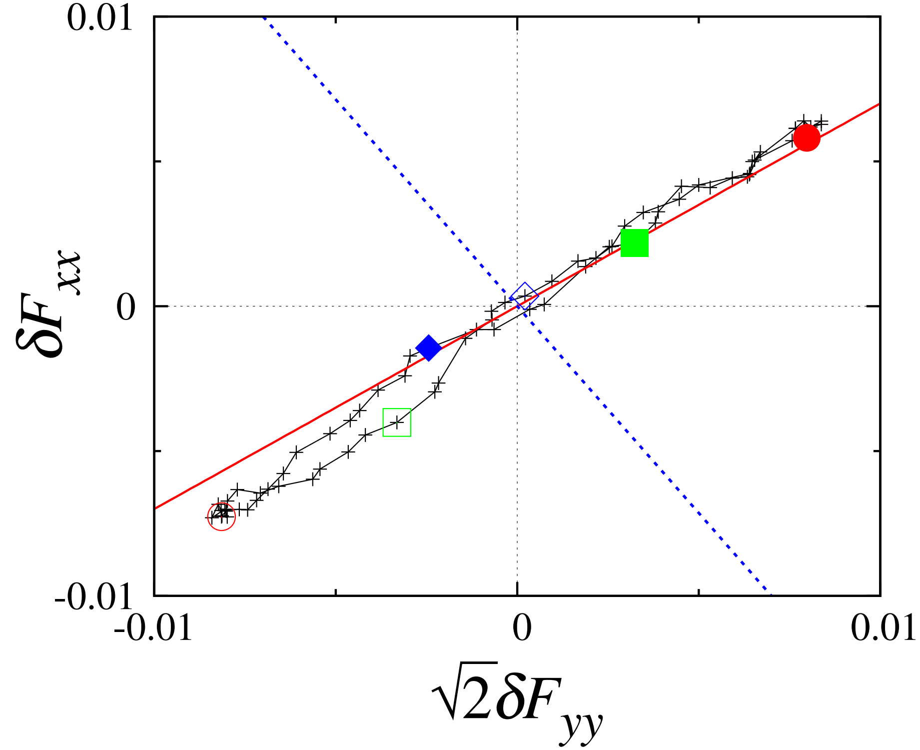


Continuum Theory

Predictive power – large strain shear MACRO

=> Failure/yield loci/surfaces … work in progress …





Rheology: So much for the jamming point …

Response: jamming "point" moves!

- slow for ISO => increase => consolidation
- fast for DEV => decrease ⇔ **dilatancy**

Micro-structure: Packing "efficiency" & anisotropy

Fluid with solid features vs. flowing solid

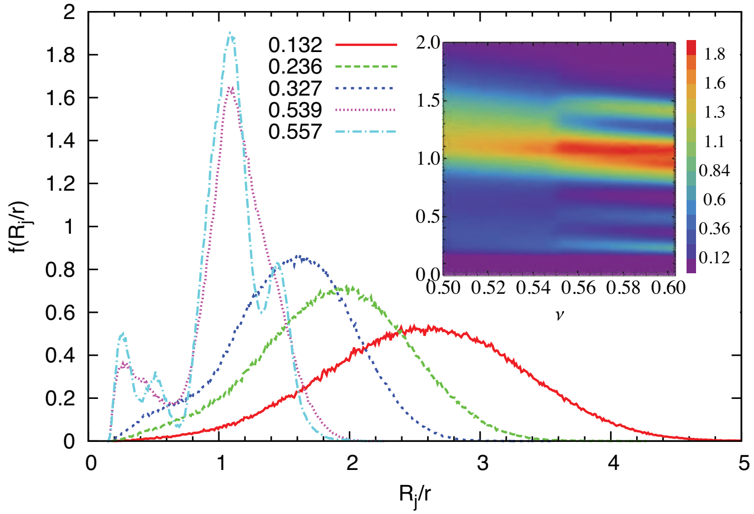
There is not just one phase-diagram ☹

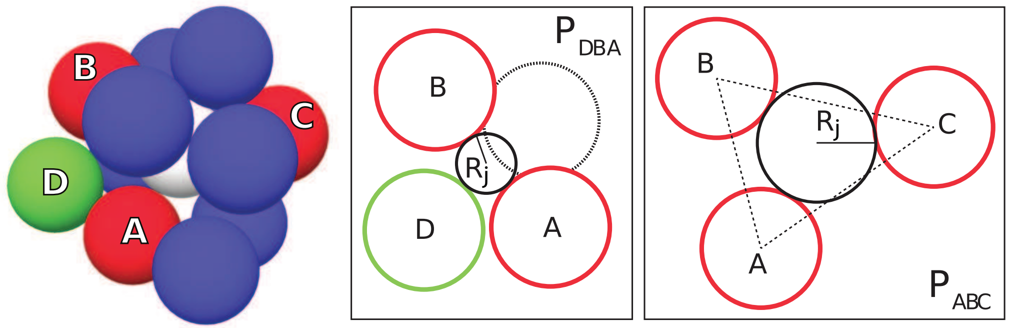
All mechanisms **without friction** (colloids/glass)

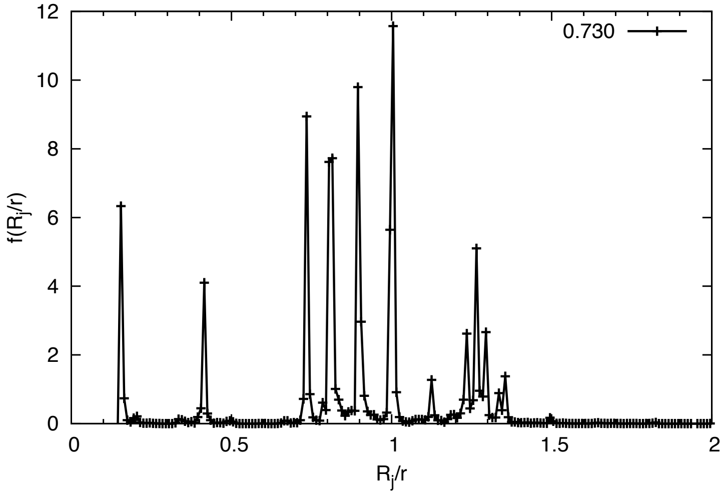
1 – friction/material changes regime/values

2 - re-entrance = shear-jamming/-thickening

Fluid with solid features ⇔ microstructure



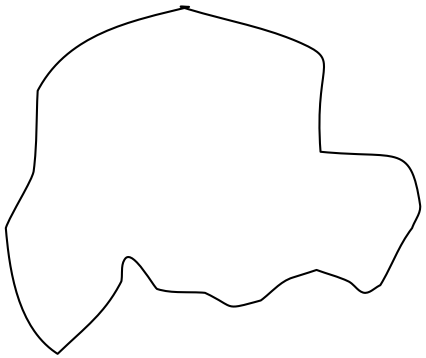




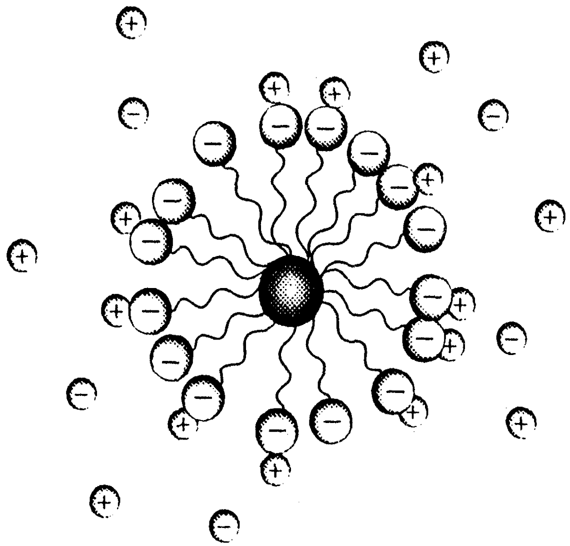
channel/throat distribution
(4 particle correlation)
2D order in 3D !

V. Ogarko, N. Rivas, SL, JCP 2014

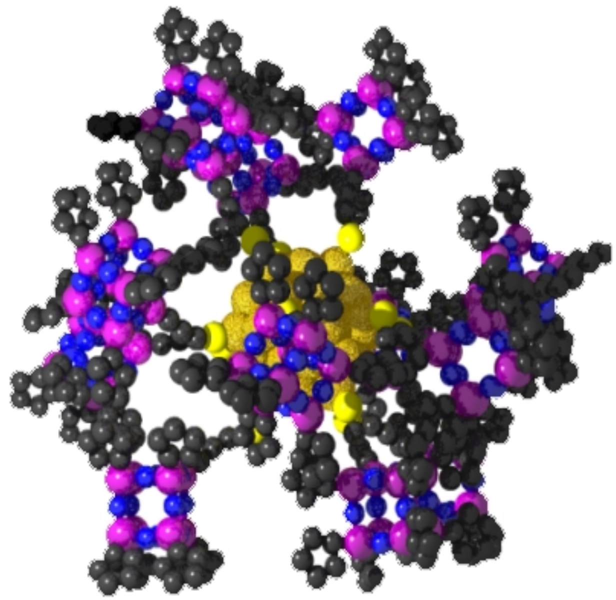
Particle Interactions



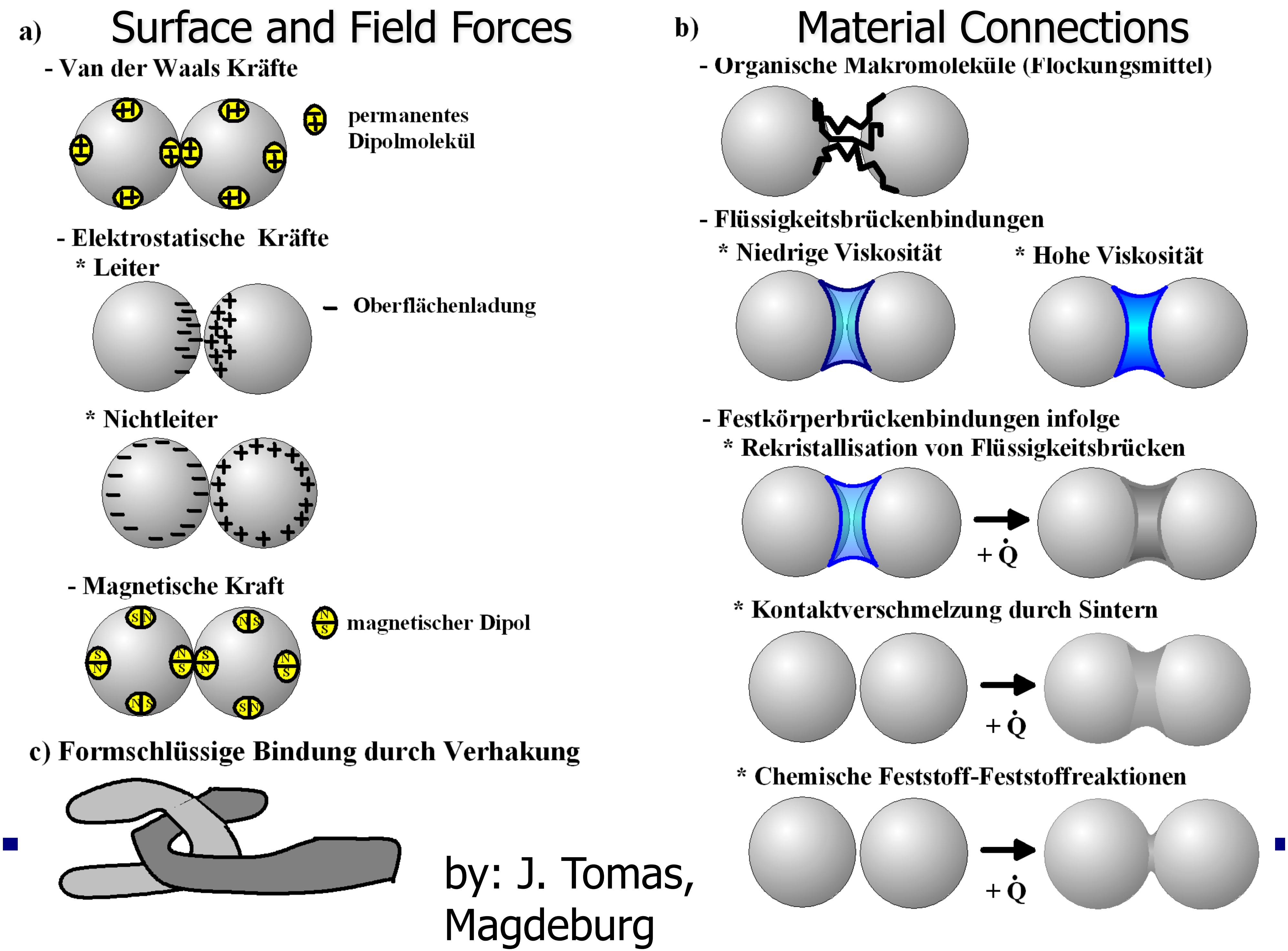
Mechanical
(d_p>10µm)



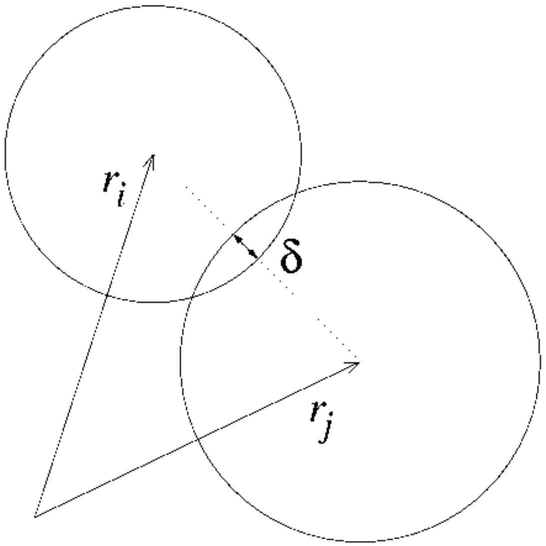
Chemical
(10nm<d_p<10µm)



Atomic Cluster
(d_p<10nm)


a) Surface and Field Forces
- Van der Waals Kräfte
permanentes Dipolmolekül
- Elektrostatische Kräfte
* Leiter
Oberflächenladung
* Nichtleiter
- Magnetische Kraft
magnetischer Dipol
c) Formschlüssige Bindung durch Verhakung
b) Material Connections
- Organische Makromoleküle (Flockungsmittel)
- Flüssigkeitsbrückenbindungen
* Niedrige Viskosität
* Hohe Viskosität
- Festkörperbrückenbindungen infolge
* Rekristallisation von Flüssigkeitsbrücken
+ Q̇
* Kontaktverschmelzung durch Sintern
+ Q̇
* Chemische Feststoff-Feststoffreaktionen
+ Q̇
by: J. Tomas, Magdeburg

Discrete particle model



Equations of motion

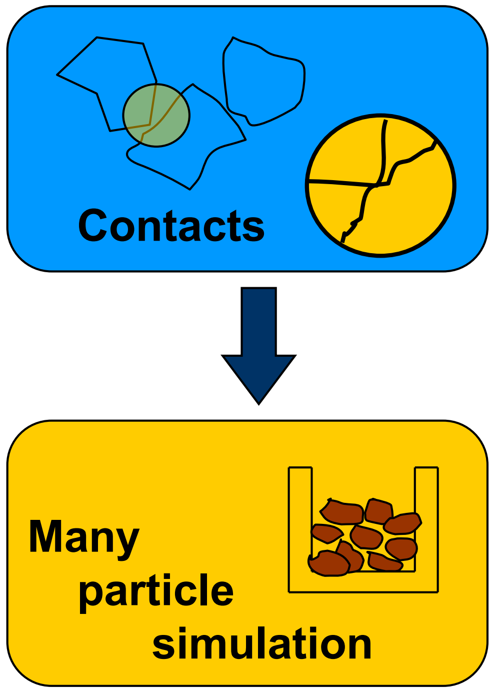
$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{f}_i \qquad I_i \frac{d\overrightarrow{\omega_i}}{dt} = \vec{t}_i$$

Forces and torques:

$$\vec{f}_i = \sum_c \vec{f}_i^{\,c} + \sum_w \vec{f}_i^{\,w} + m_i g$$

$$\vec{t}_i = \sum_c \vec{r}_i^{\,c} \times \vec{f}_i^{\,c}$$

Overlap $\quad \delta = \frac{1}{2}\left(d_i + d_j\right) - \left(\vec{r}_i - \vec{r}_j\right)\cdot \vec{n}$



How to model Contacts?

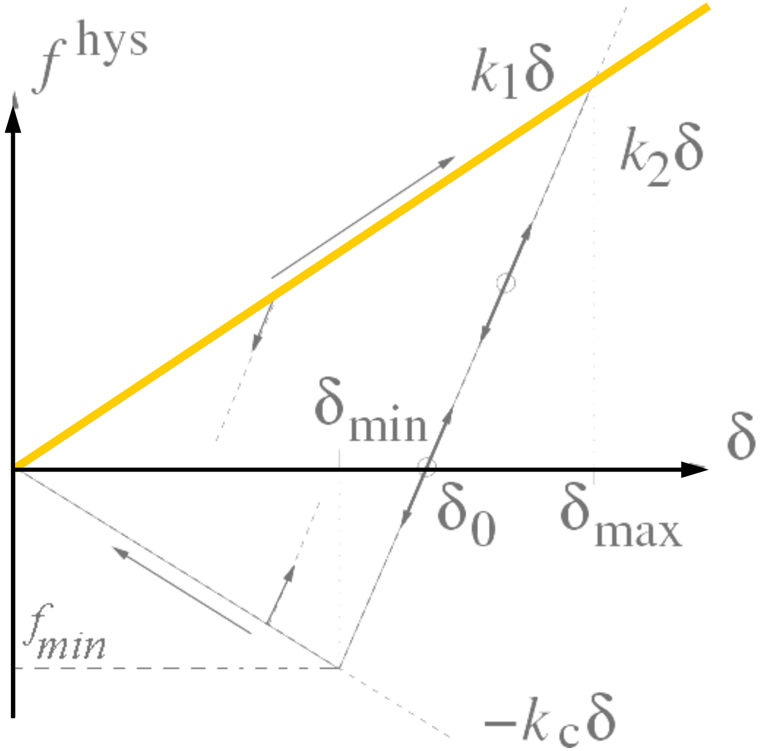
Atomistic/Molecular ...

Continuum theory + Contact Mechanics

Experiments (Nano-Ind., AFM, Mech., HSMovies)

Contact Modeling

- Full/All Details ... too much!
- **Mesoscopic type Models**
- (Over-)Simplified Models



Linear Contact model

- (really too) simple ☺
- linear
- very easy to implement

$$f_i^{hys} = \begin{cases} k_1\delta & \text{for un-/re-loading} \\ & \end{cases}$$

Linear Contact model

$$f_i = -m_{ij}\ddot{\delta} = k\delta + \gamma\dot{\delta}$$

$$k\delta + \gamma\dot{\delta} + m_{ij}\ddot{\delta} = 0$$

$$\frac{k}{m_{ij}}\delta + 2\frac{\gamma}{2m_{ij}}\dot{\delta} + \ddot{\delta} = 0$$

$$\boxed{\omega_0^2\delta + 2\eta\dot{\delta} + \ddot{\delta} = 0}$$

- really simple ☺
- linear, analytical
- very easy to implement

$$\delta(t) = \frac{v_0}{\omega}\exp(-\eta t)\sin(\omega t)$$

$$\dot{\delta}(t) = \frac{v_0}{\omega}\exp(-\eta t)\left[-\eta\sin(\omega t) + \omega\cos(\omega t)\right]$$

elastic freq. $\omega_0 = \sqrt{k/m_{ij}}$

eigen-freq. $\omega = \sqrt{\omega_0^2 - \eta^2}$

visc. diss. $\eta = \dfrac{\gamma}{2m_{ij}}$

contact duration $\boxed{t_c = \pi/\omega}$

restitution coefficient $r = -\dfrac{v(t_c)}{v_0} = \exp(-\eta t_c)$

http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf

Time-scales

time-step $\Delta t <= {}^{t_c}\!/_{50}$

contact duration $\boxed{t_c = {}^{\pi}\!/_{\omega}}$

$t_n < t_c$

different sized particles

$t_c^{large} > t_c^{small}$

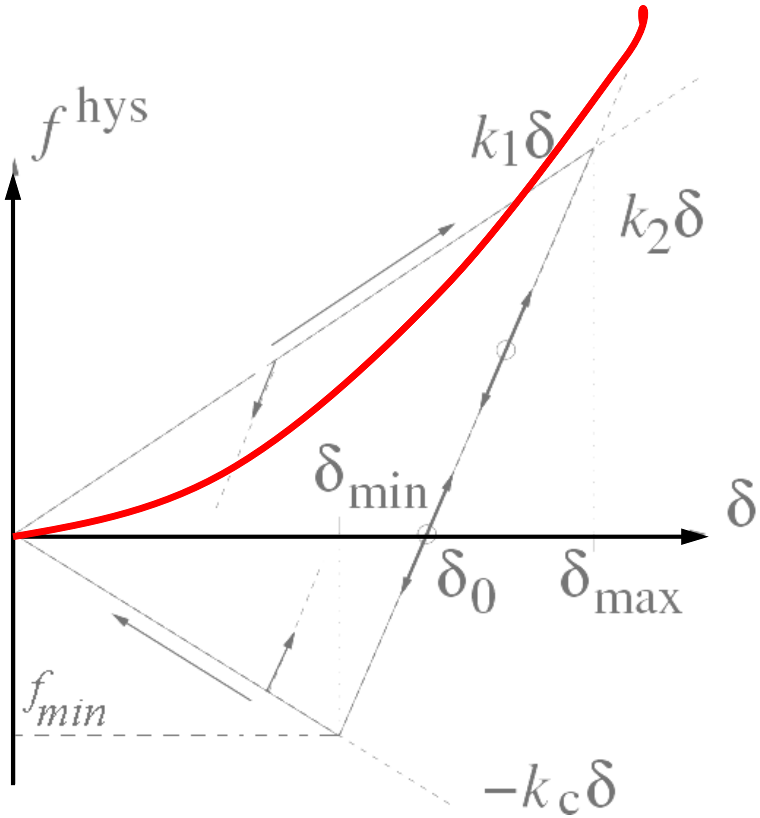
time between contacts

$t_n > t_c$

sound propagation $N_L t_c$ ... with number of layers N_L

experiment T

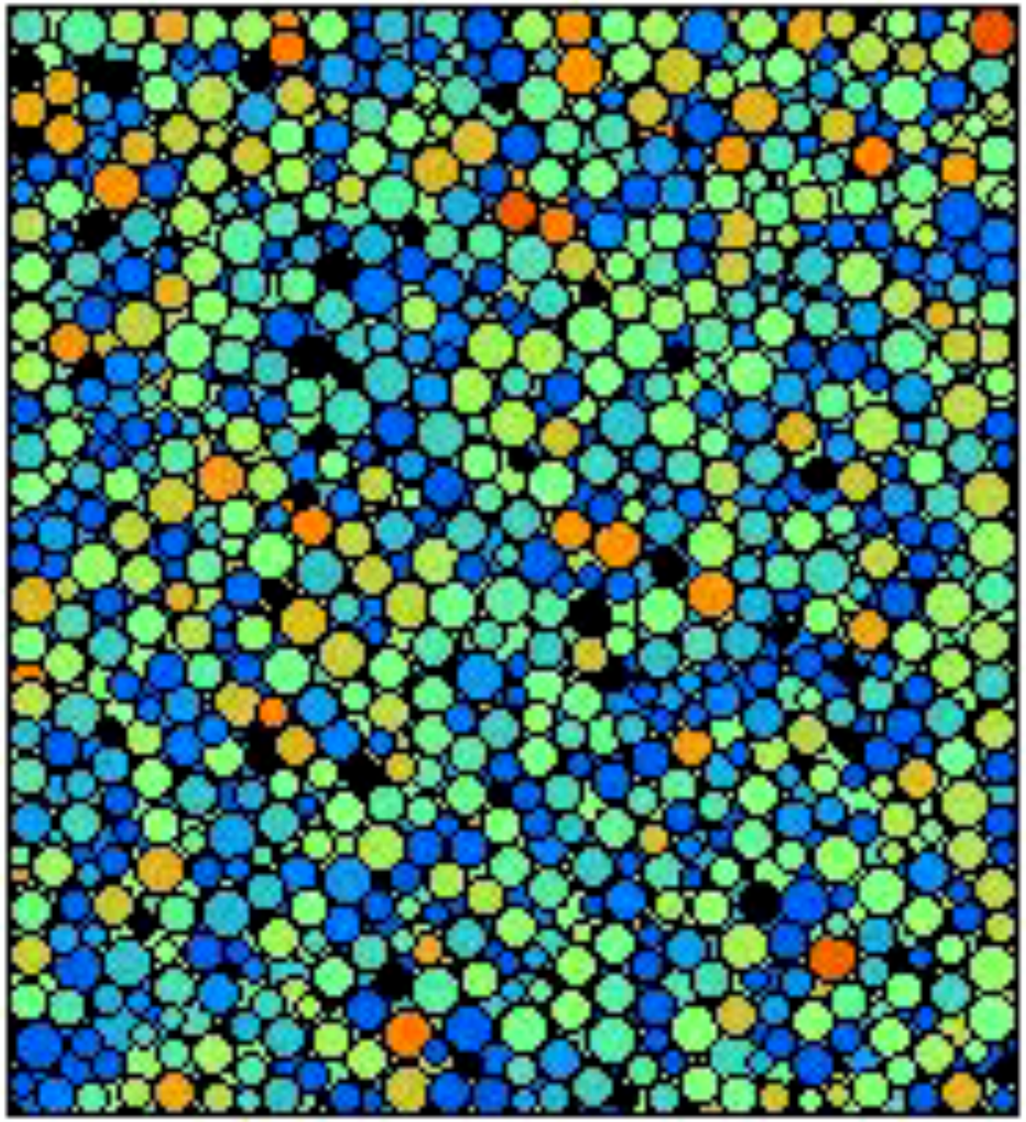
http://www2.msm.ctw.utwente.nl/sluding/PAPERS/coll2p.pdf



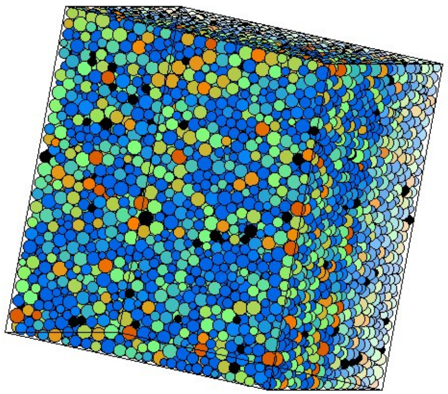
Hertz Contact model

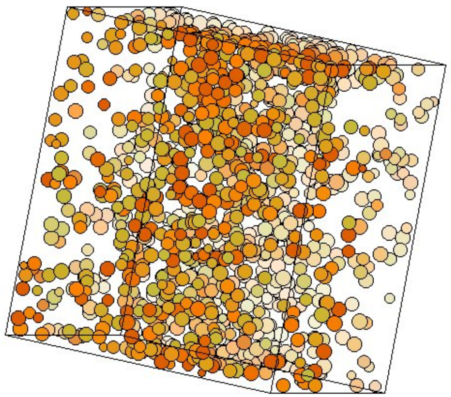
- **simple ☺**
- **non-linear**
- **easy to implement**

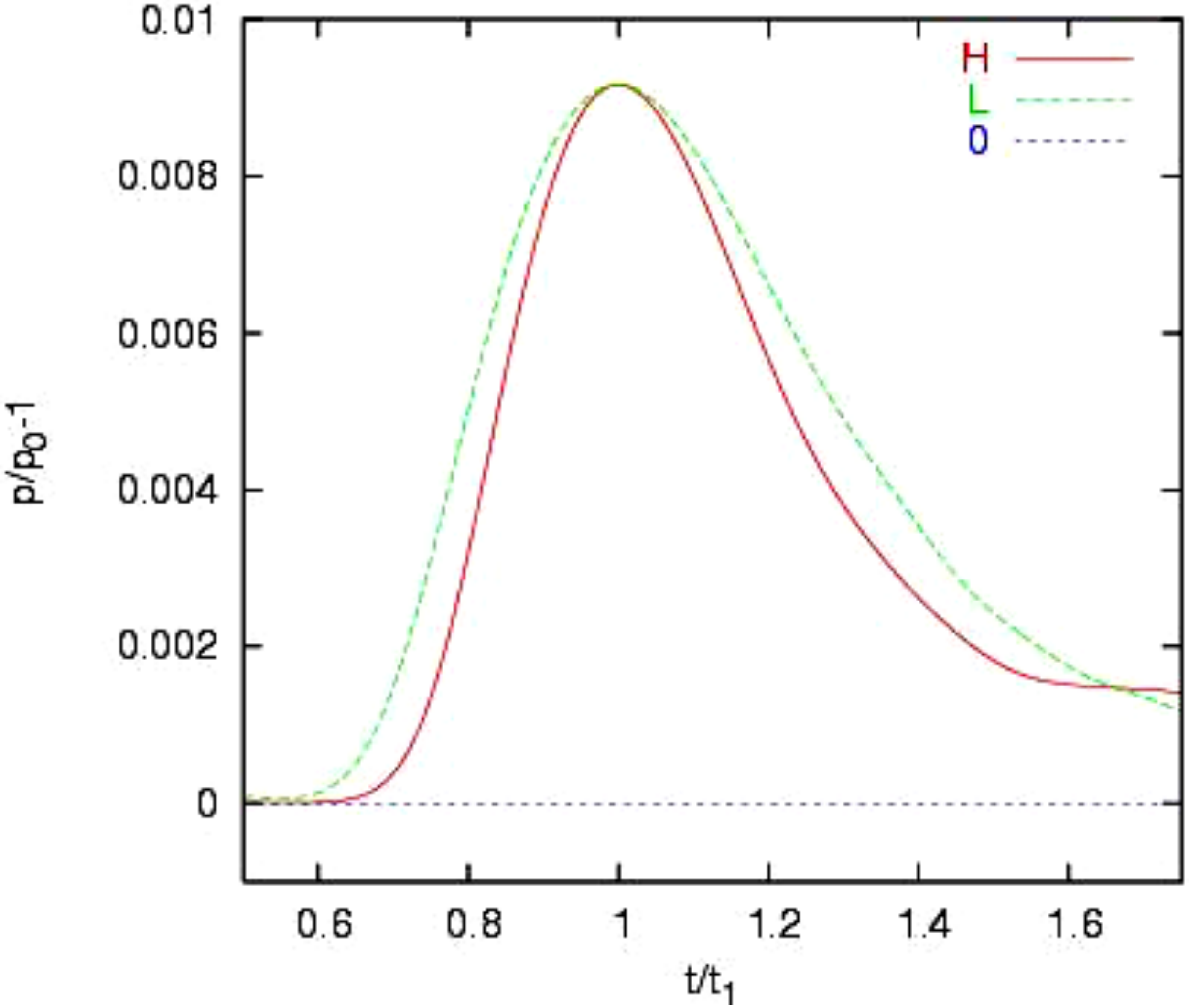
$$f_i^{hys} = \begin{cases} k_1 \delta^{3/2} & \text{for un-/re-loading} \\ & \\ & \end{cases}$$



Sound







P-wave shape and speed

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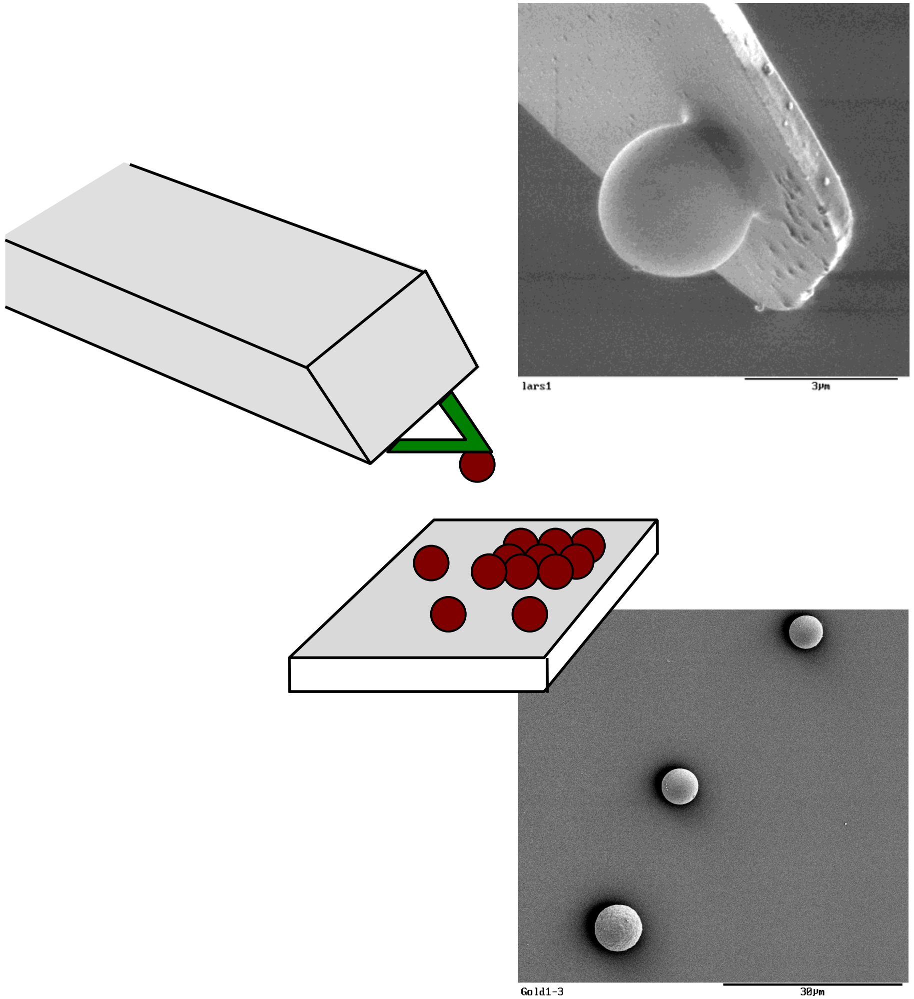
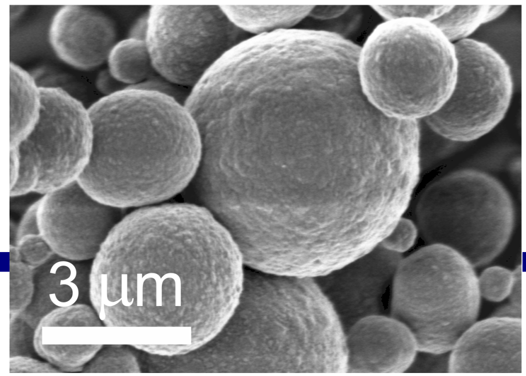
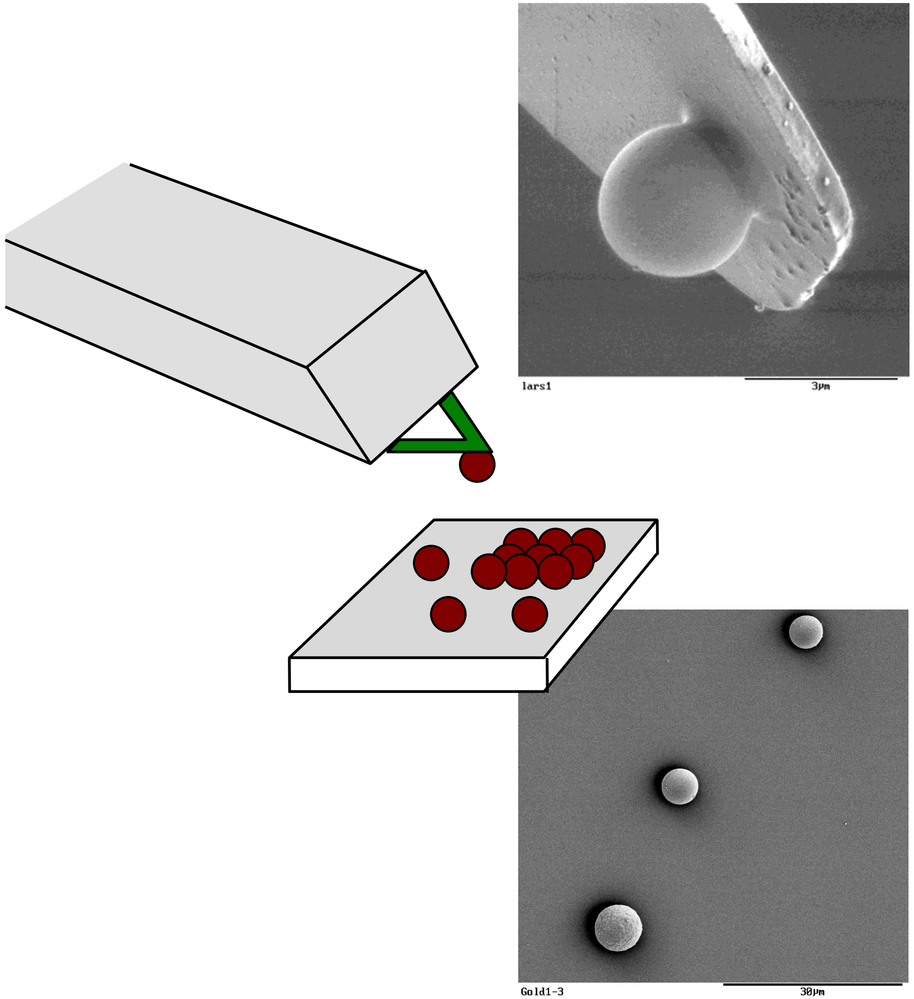
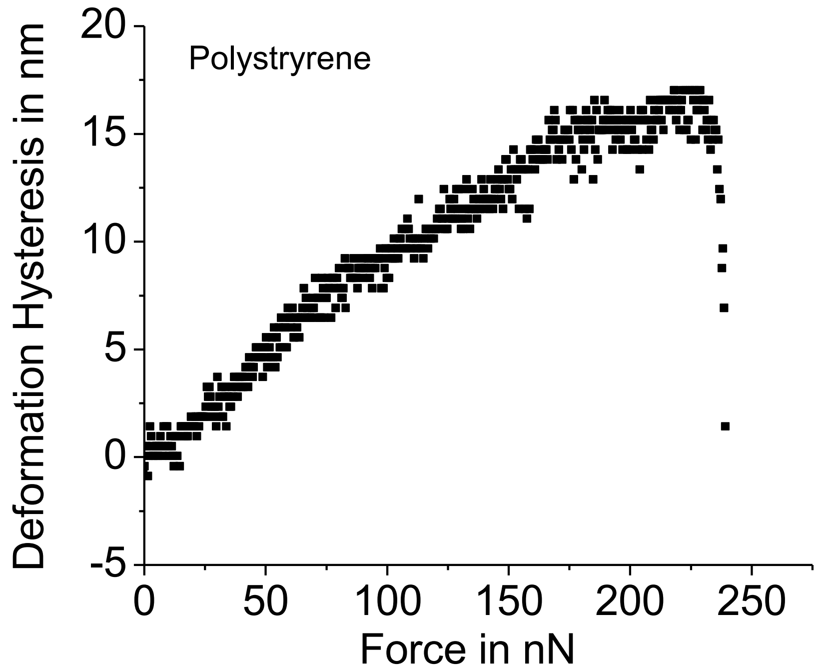
Contact force measurement (AFM)

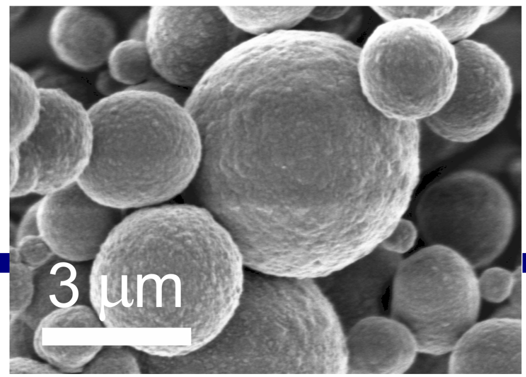




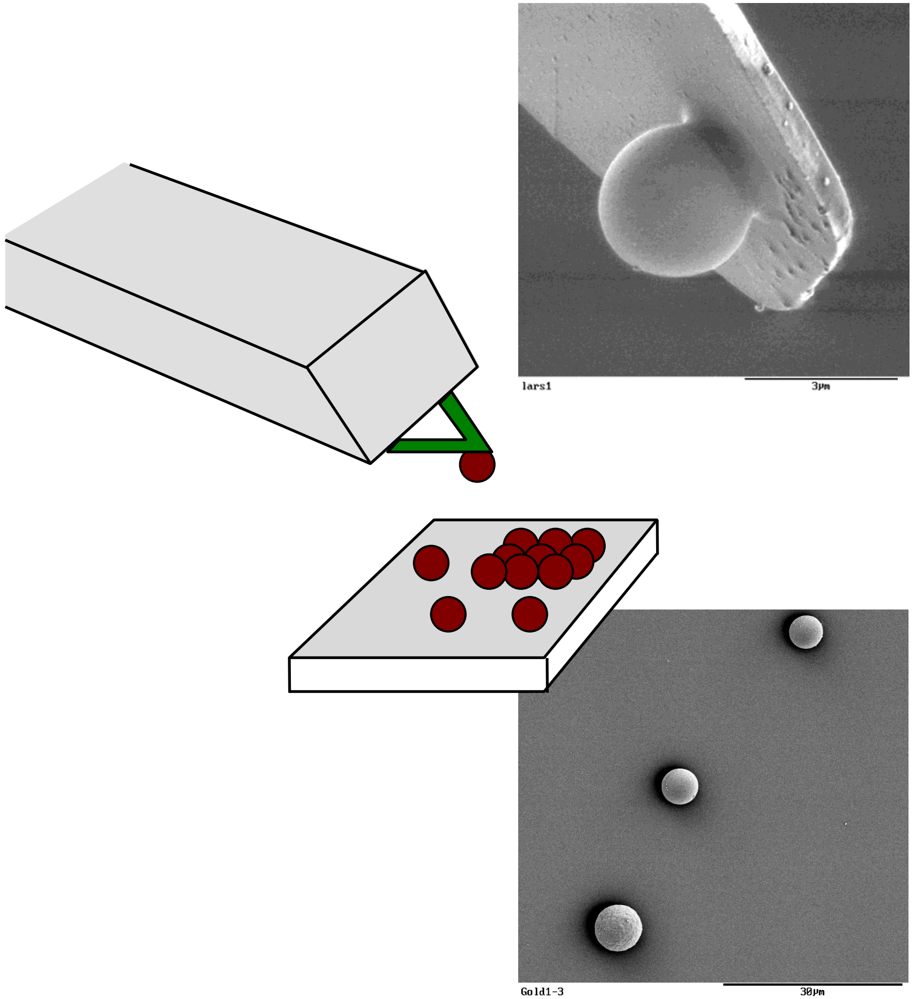
Contact force measurement (AFM)

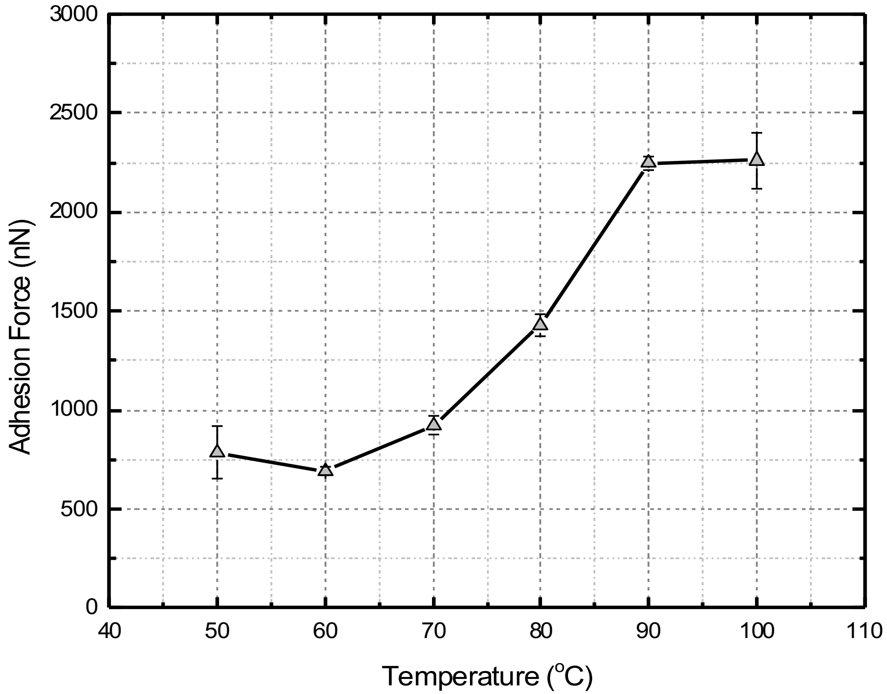


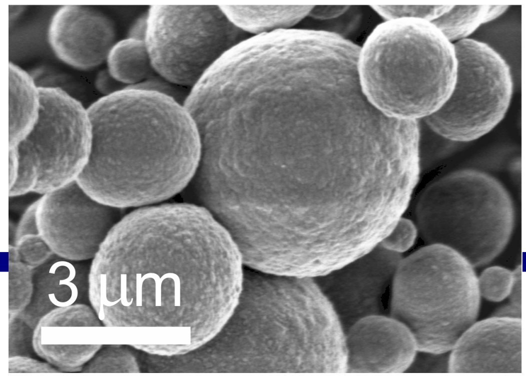




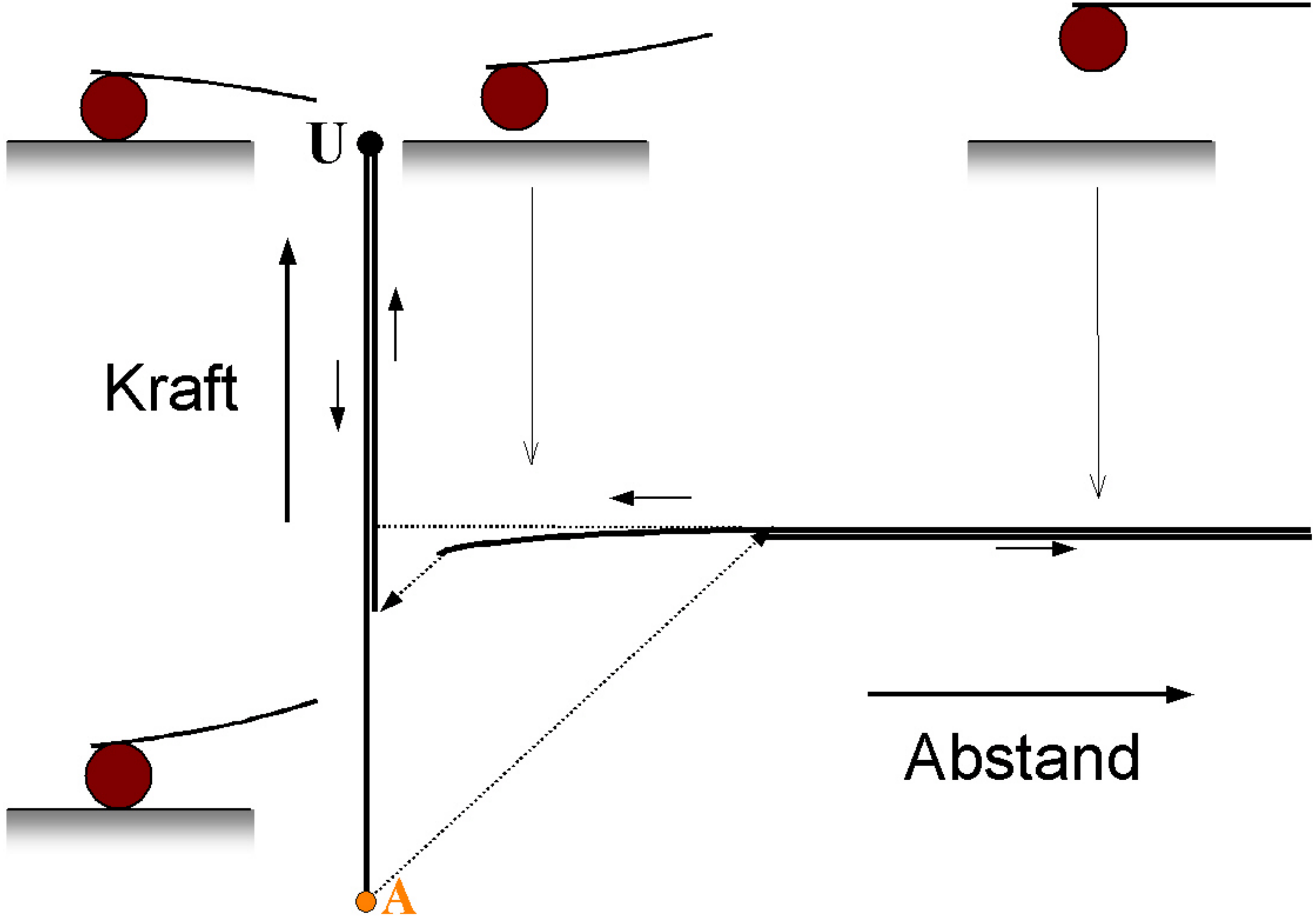
Contact force measurement (AFM)



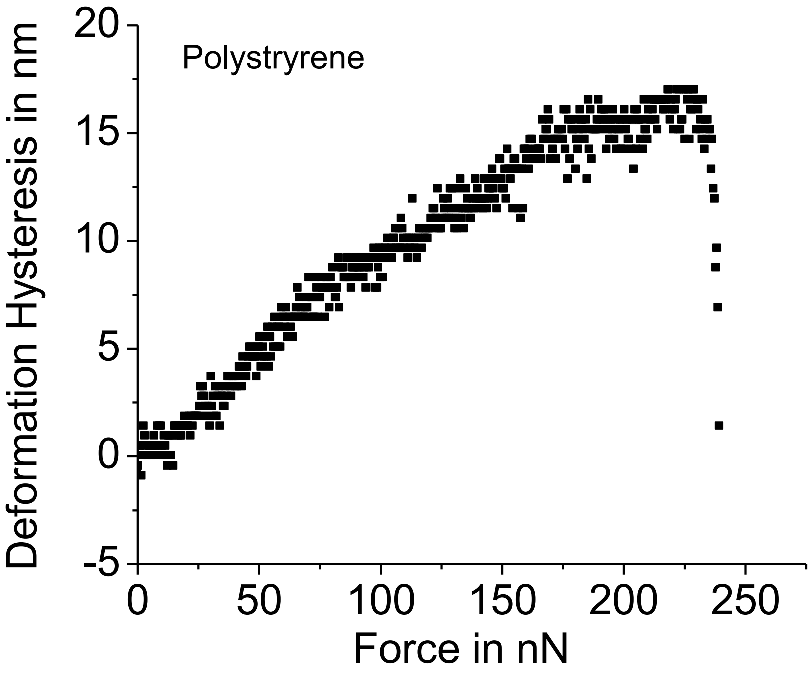


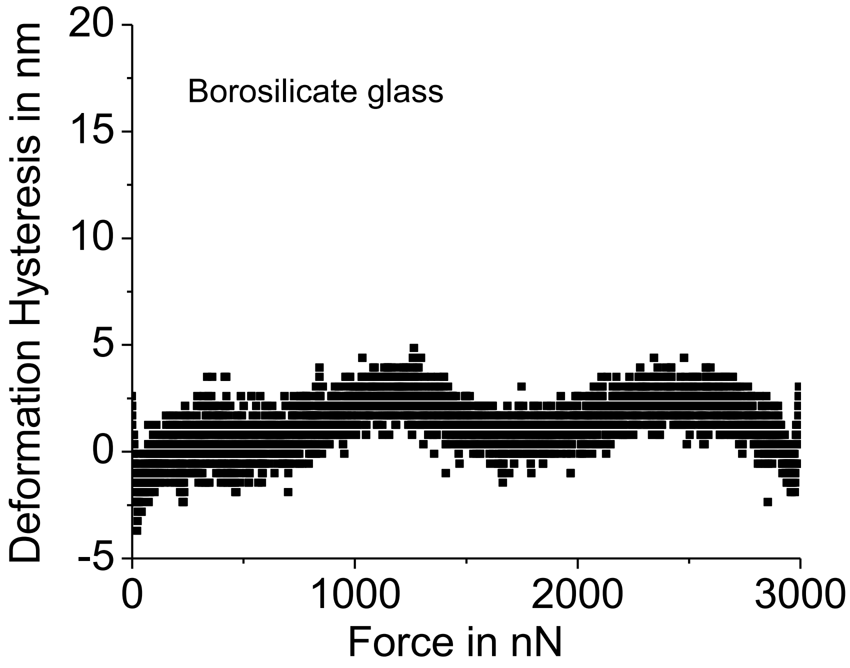


Contact Force Measurement



Hysteresis (plastic deformation)



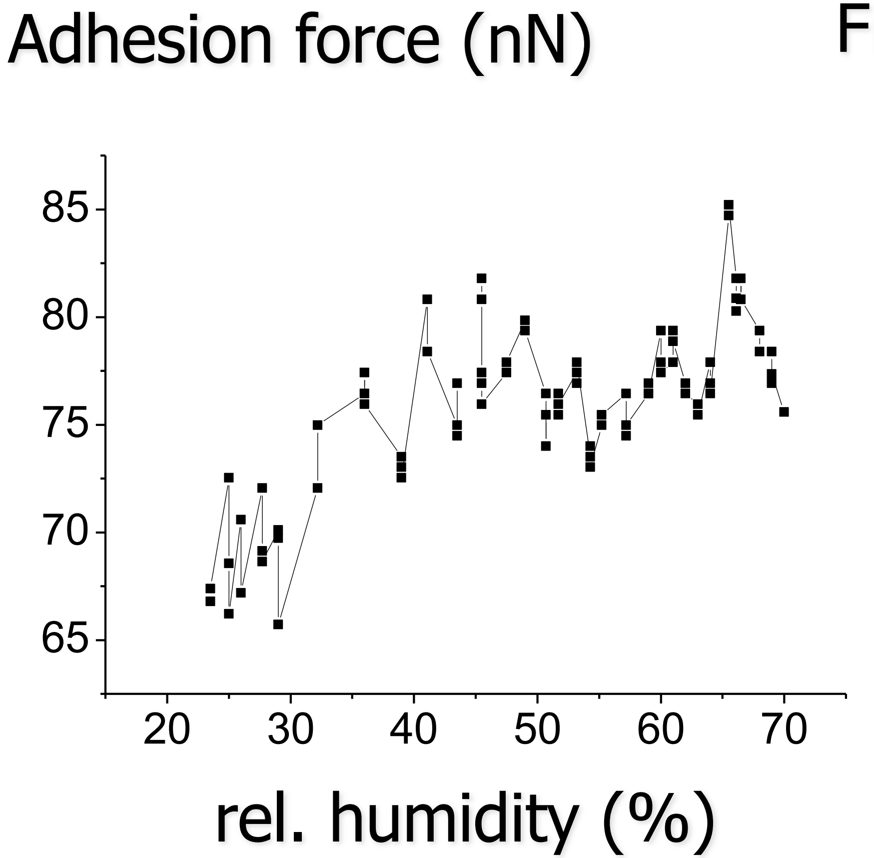


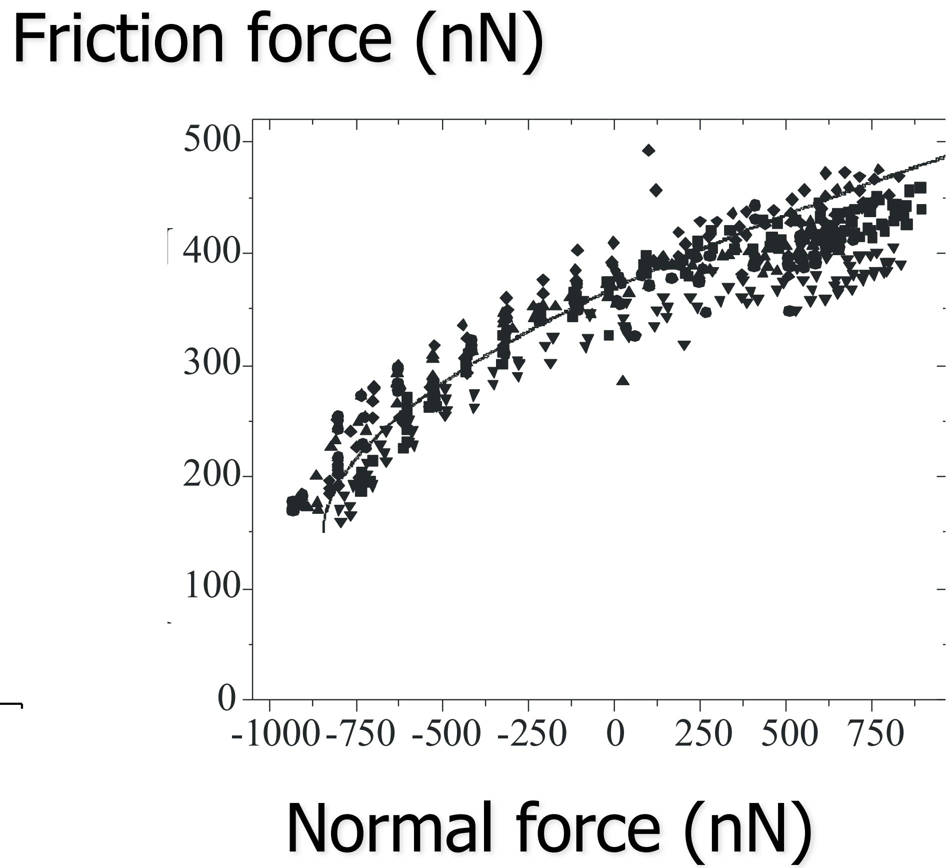
Collaborations:

MPI-Polymer Science (Butt et al.)

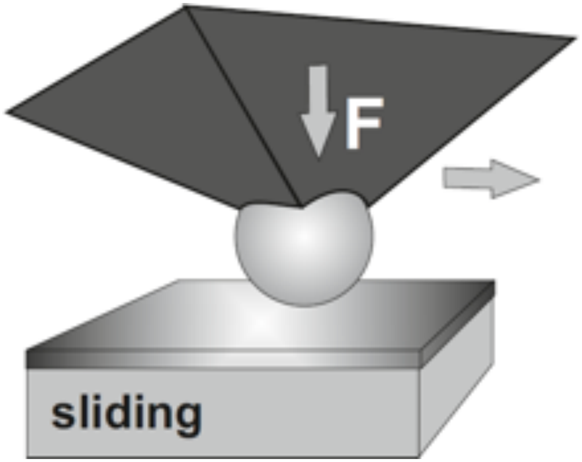
Contact properties via AFM

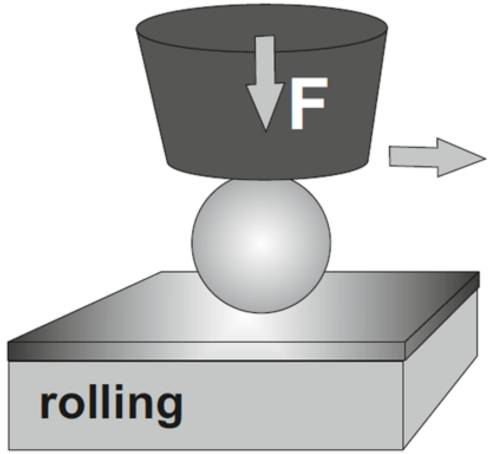
Adhesion and Friction

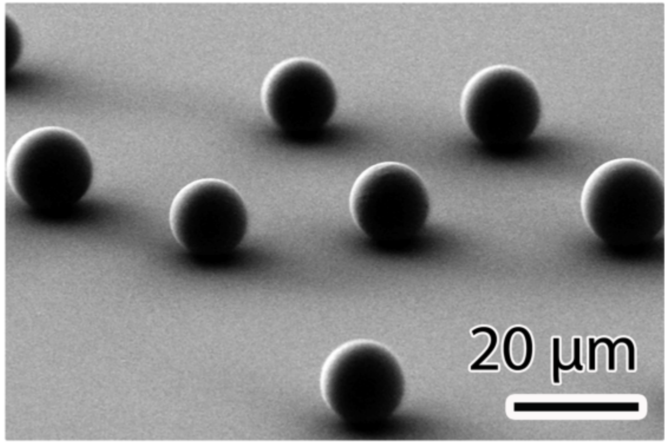


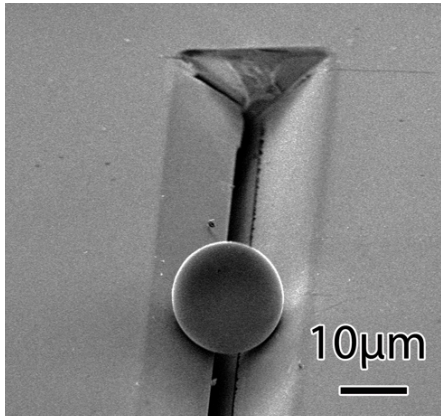


Nano-indenter -> contacts at microscale

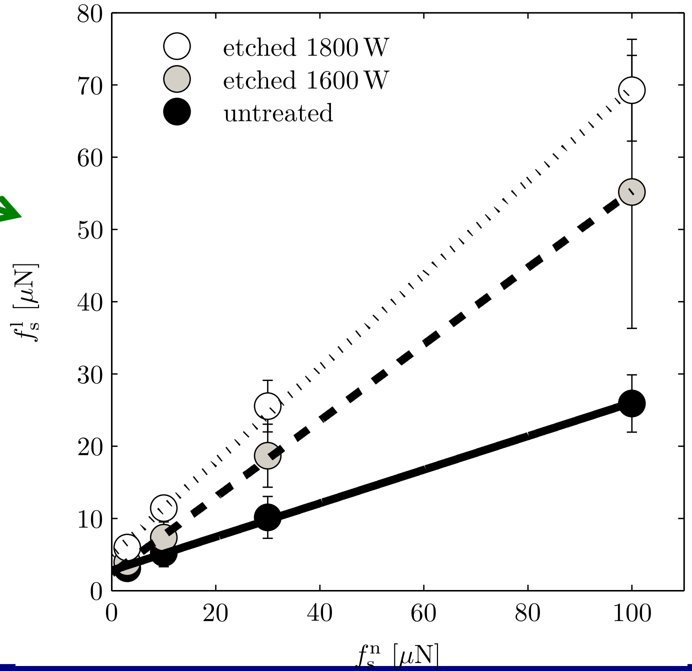






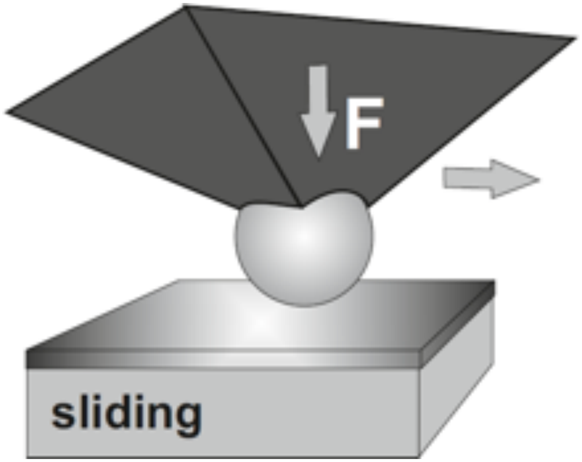


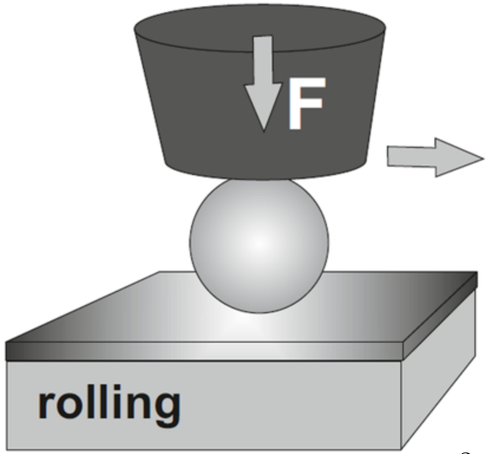
torsion
+rolling

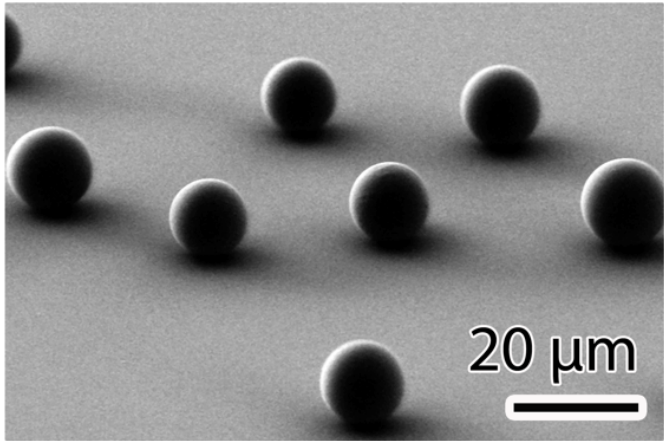


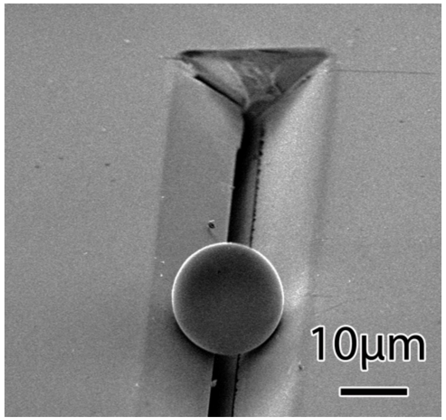
R. Fuchs, T. Weinhart, et al. Granular Matter, 2014

Nano-indenter -> contacts at microscale

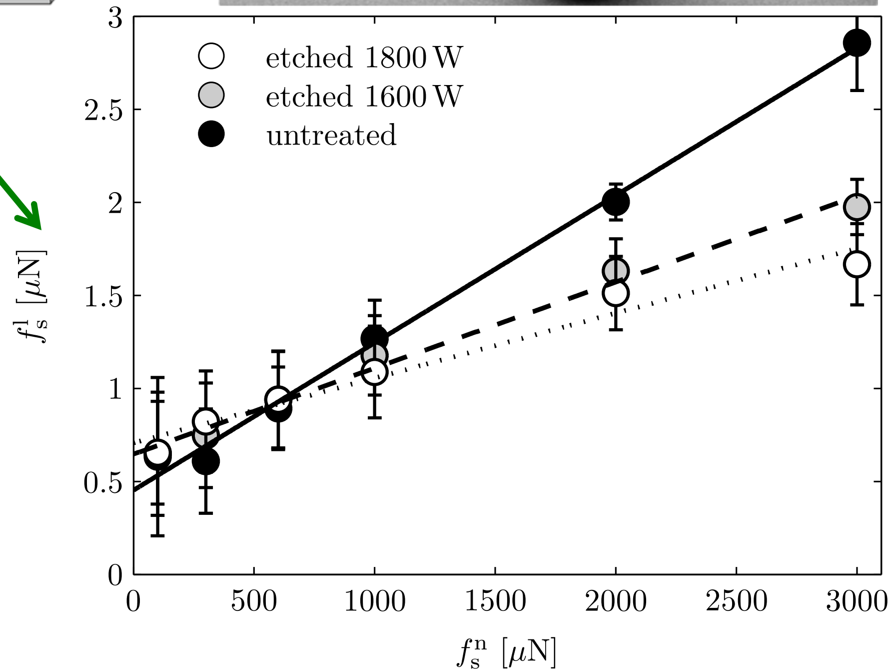






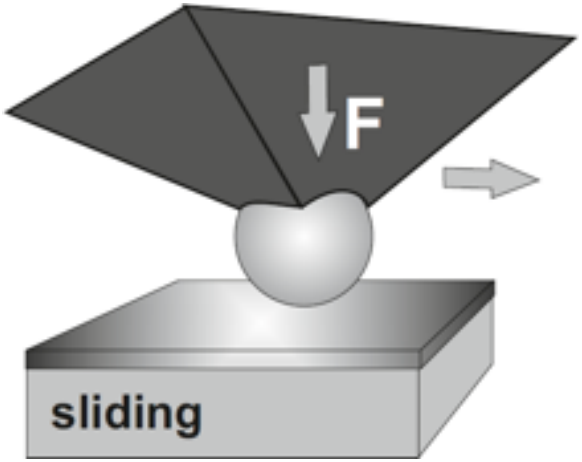


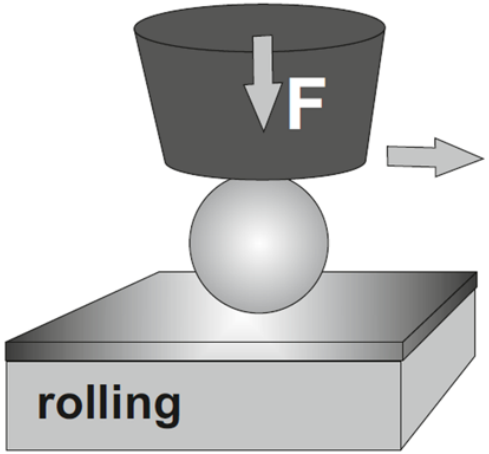
torsion
+rolling

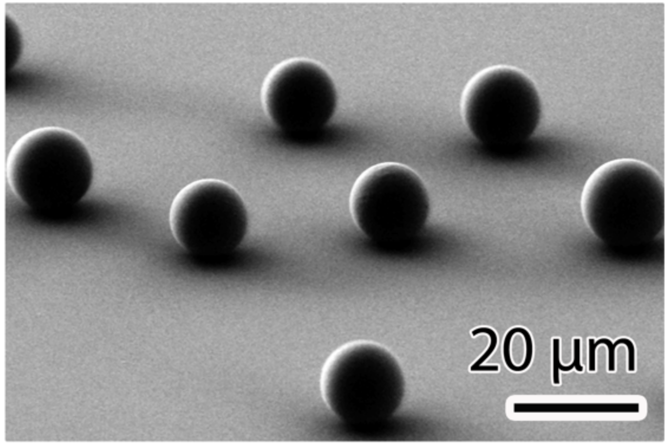


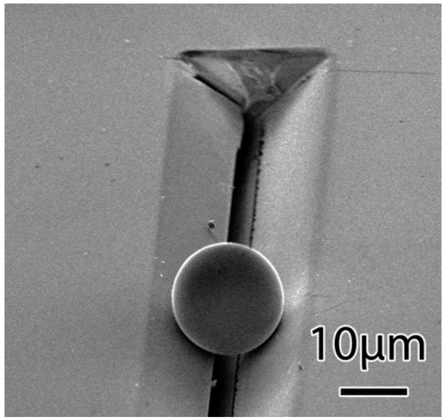
R. Fuchs, T. Weinhart, et al. Granular Matter, 2014

Nano-indenter -> contacts at microscale

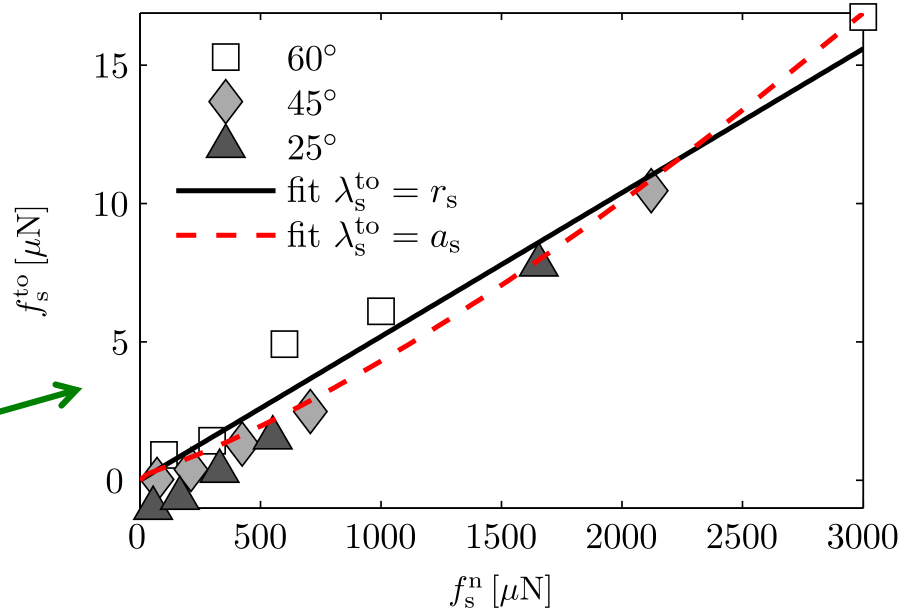






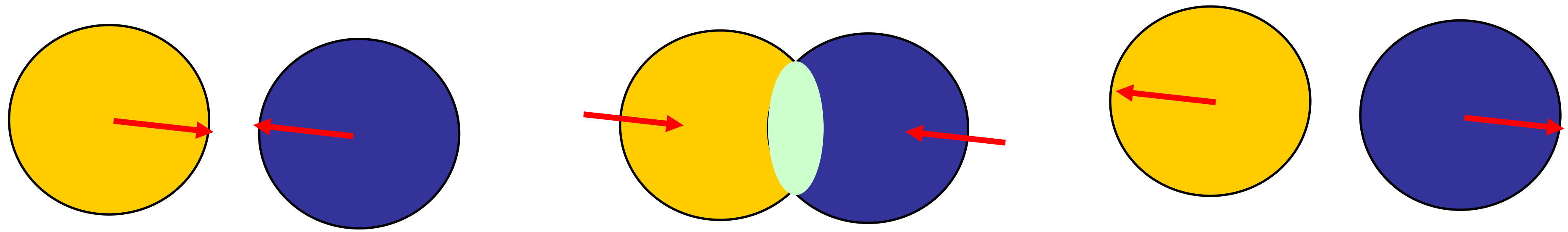


torsion
+rolling

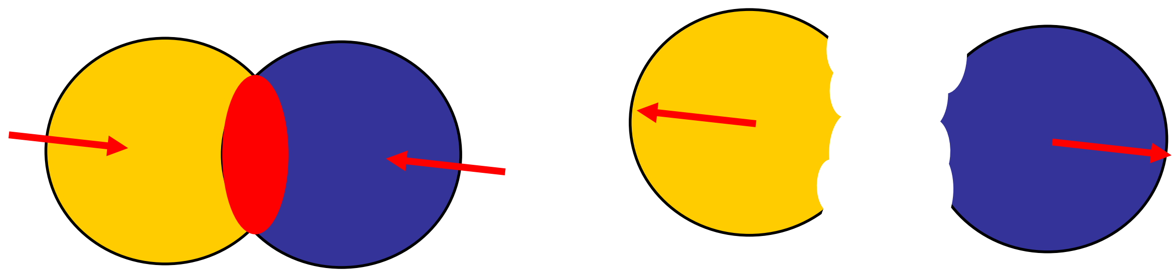


R. Fuchs, T. Weinhart, et al. Granular Matter, 2014

Elastic spheres



Elasto-plastic spheres



Before During

After

Contacts

1. loading

transition to stiffness: k_2

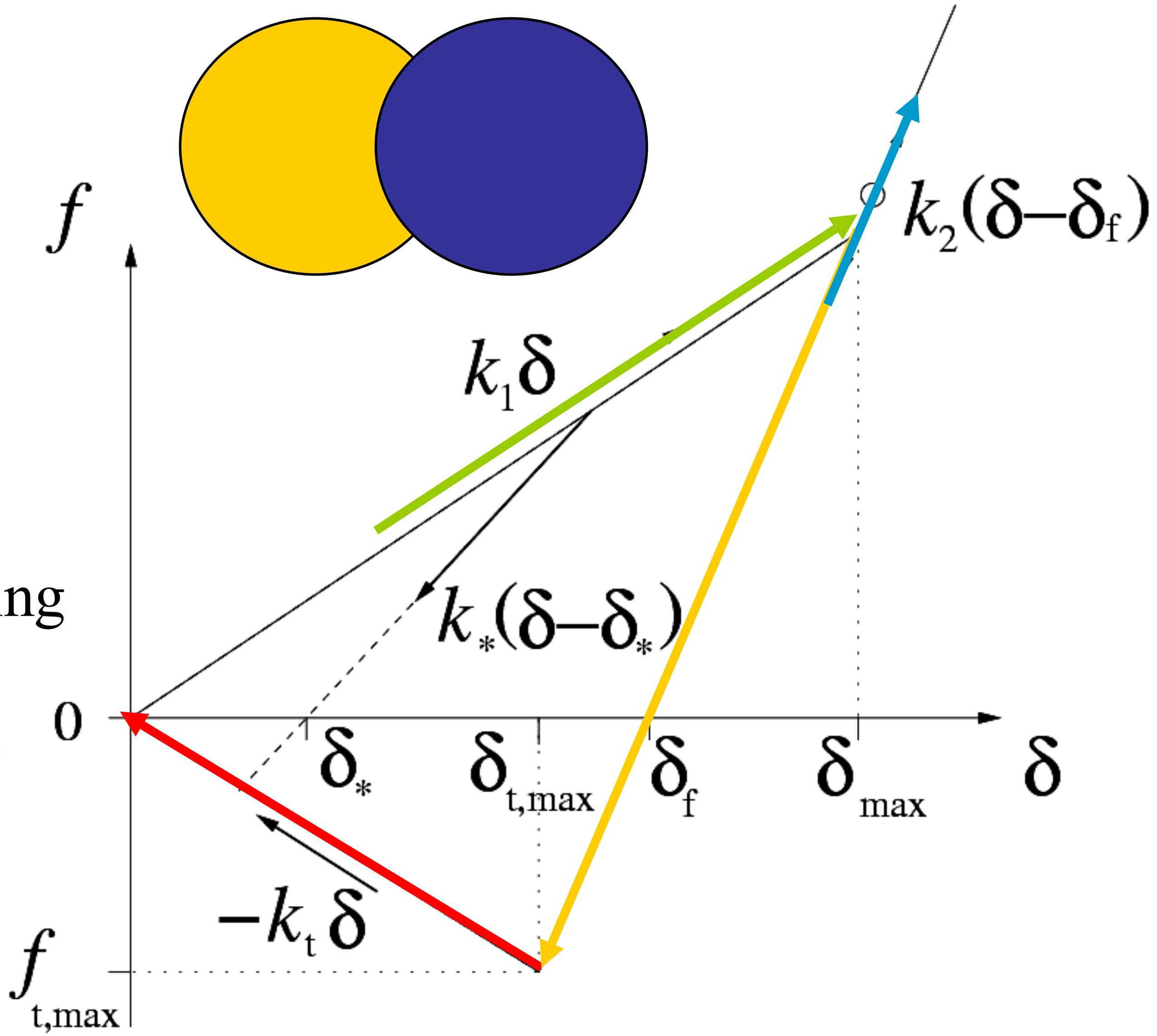
2. unloading

3. re-loading

elastic un/re-loading stiffness: k_2

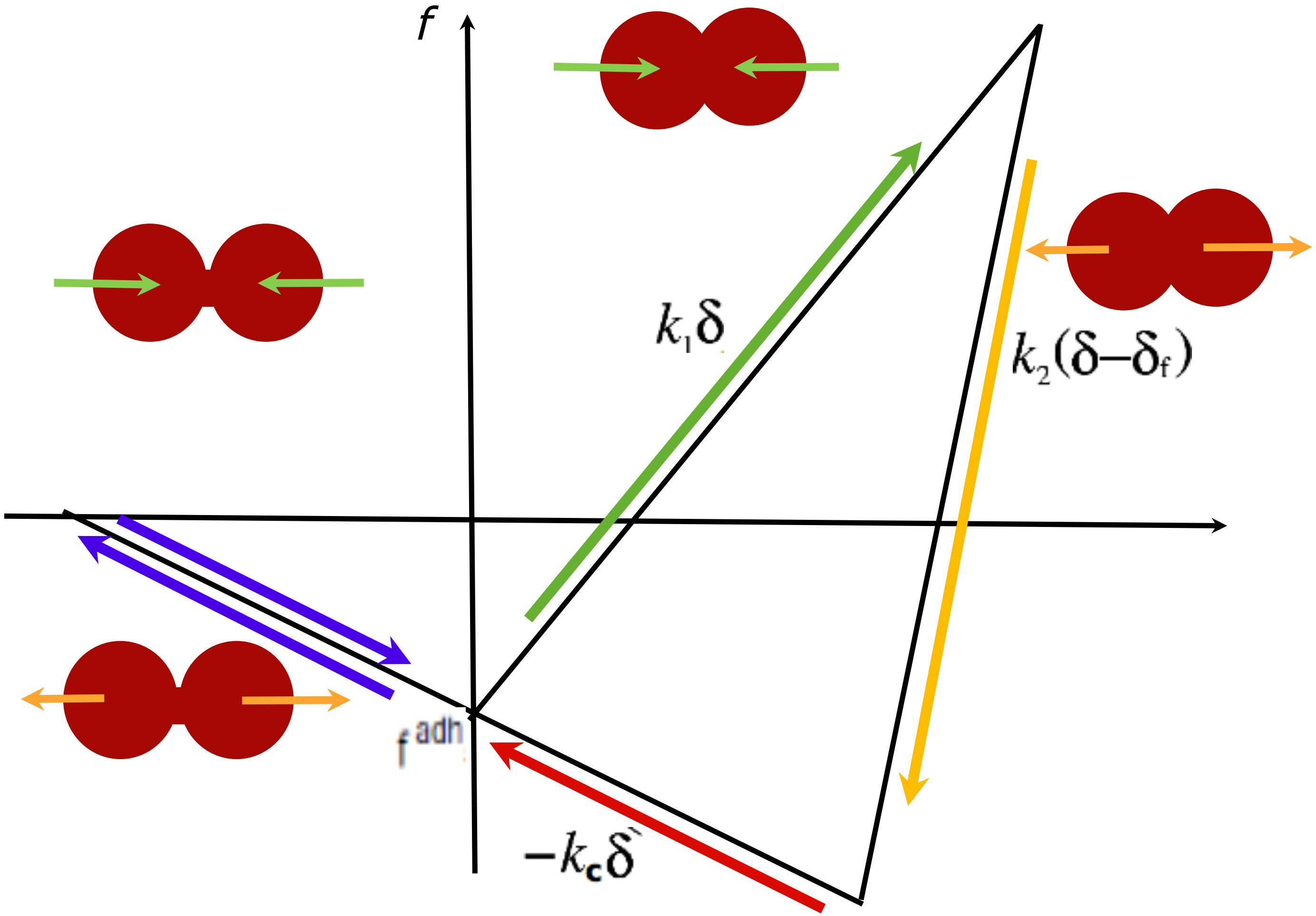
4. tensile failure

max. tensile force



Reversible elasto-plastic adhesive contacts

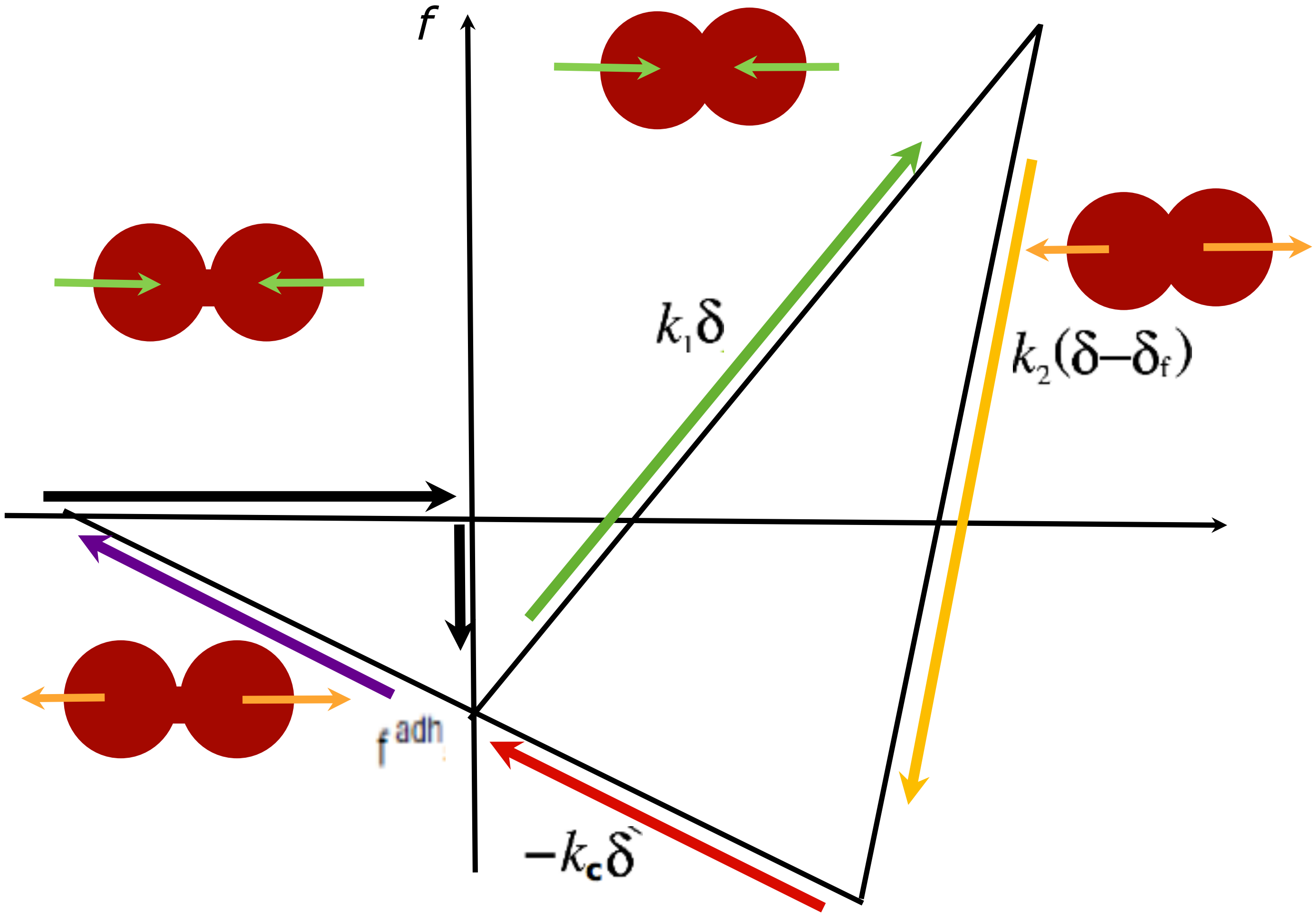
- Long range force.
- Loading
  Plastic def.
- Unloading
  "elasto-plastic"
- Re-loading
  "elastic"
- Cohesion



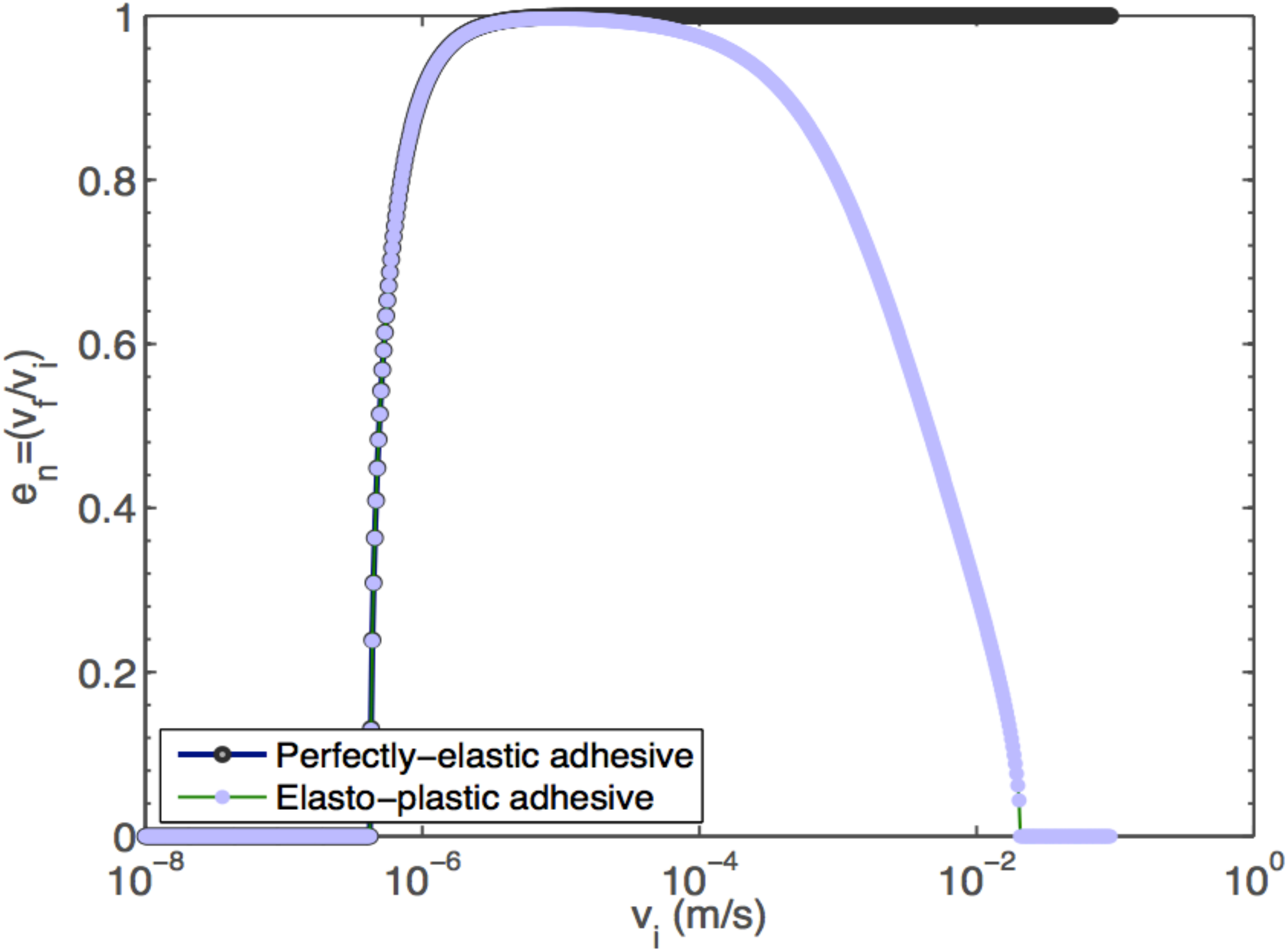
Van-der Waals type interaction.

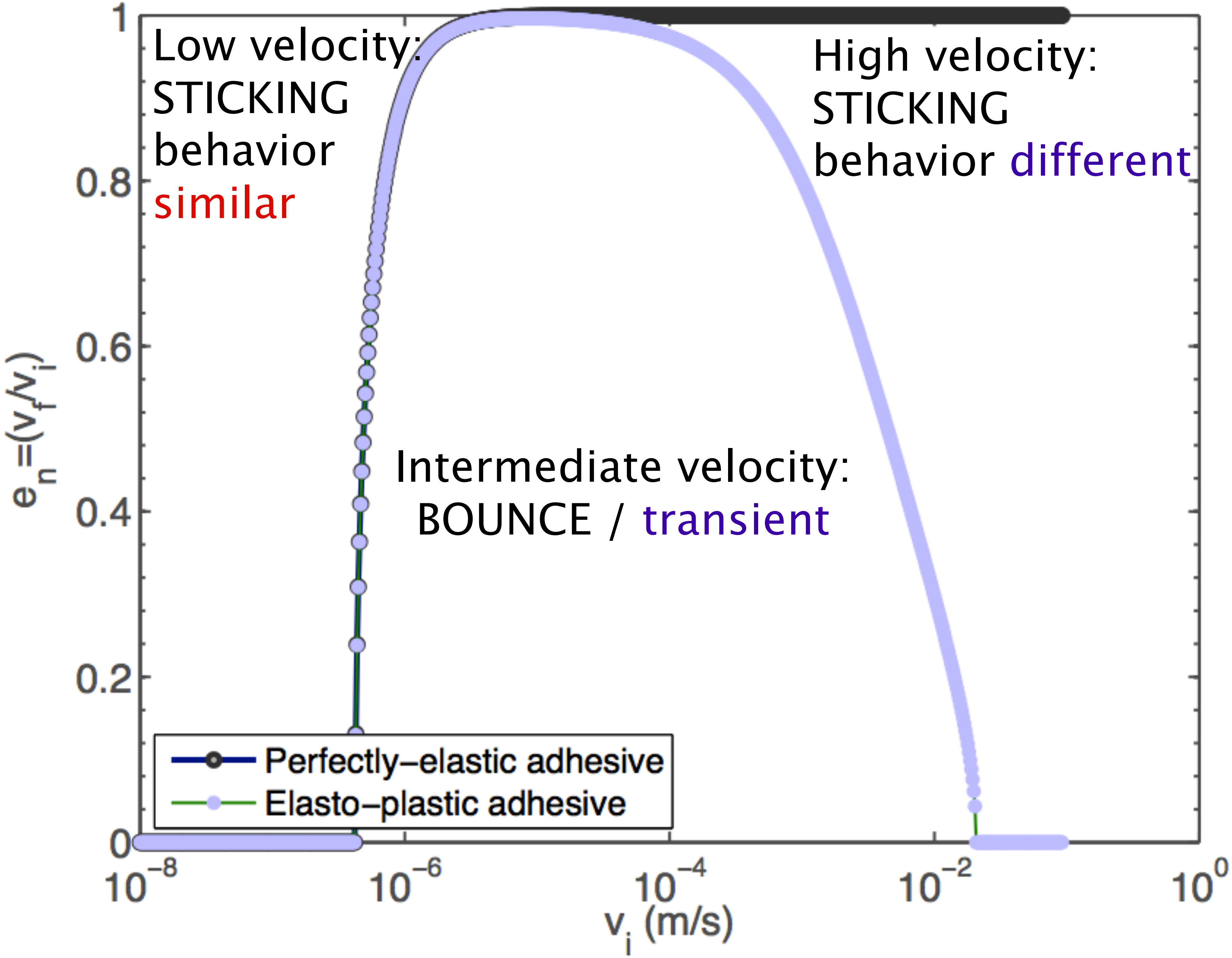
Irreversible elasto-plastic adhesive contacts

- Loading
  Plastic def.
- Unloading
  "elasto-plastic"
- Re-loading
  "elastic"
- Cohesion
- Long-range
  forces …



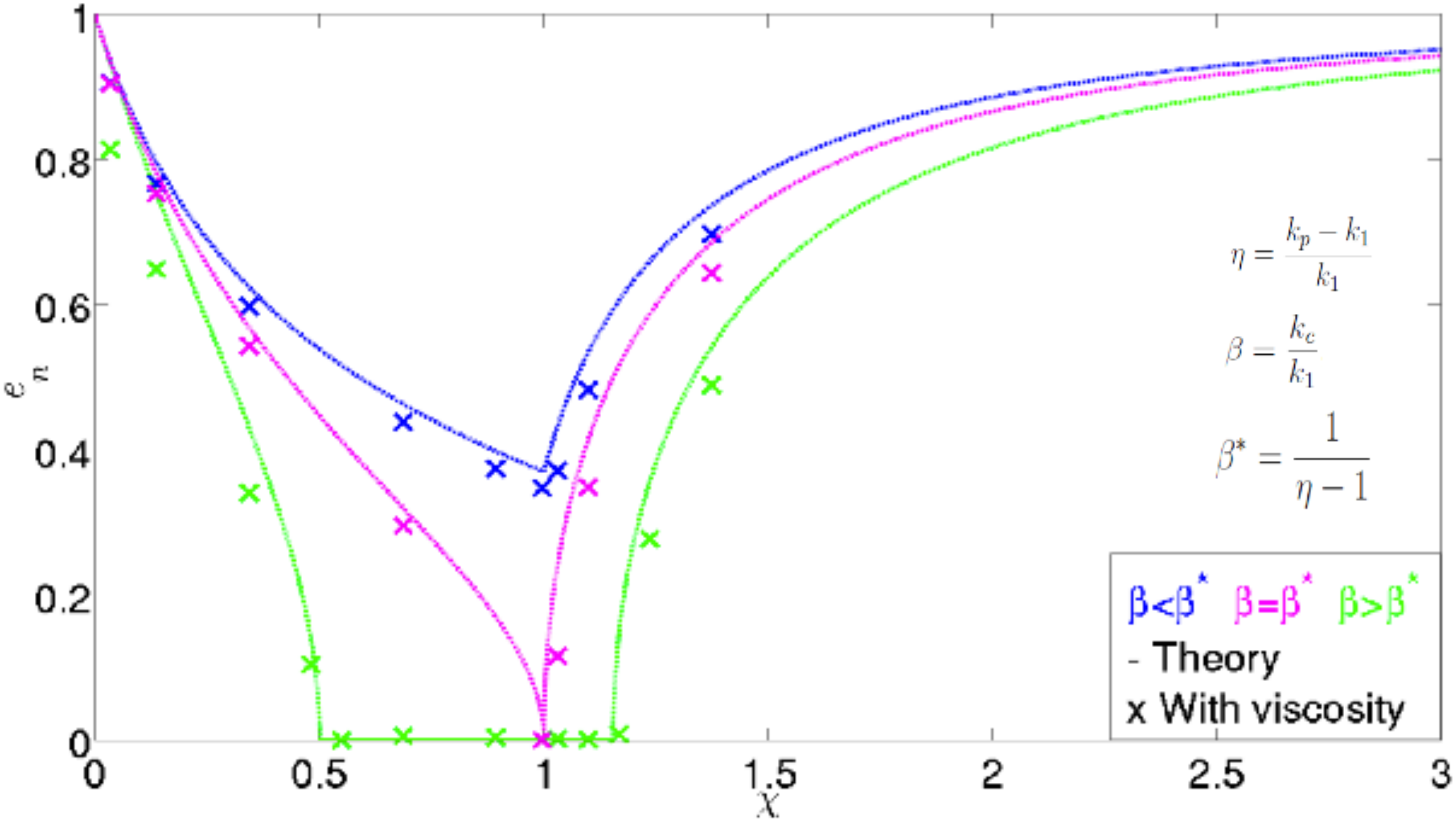
Coefficient of restitution



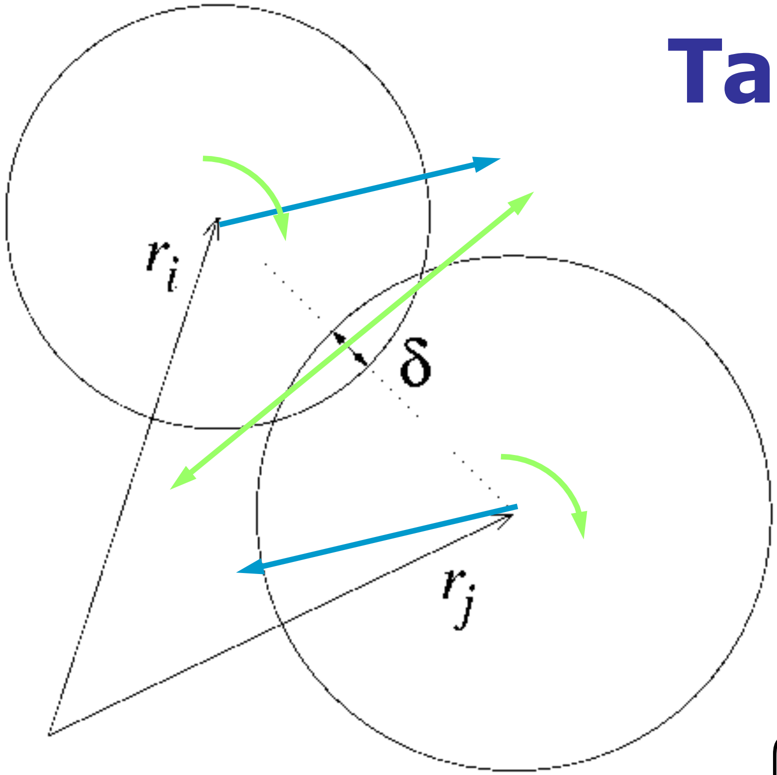


Low velocity:
STICKING
behavior
similar
High velocity:
STICKING
behavior different
Intermediate velocity:
BOUNCE / transient
Perfectly–elastic adhesive
Elasto–plastic adhesive
$e_n=(v_f/v_i)$
v_i (m/s)
0
0.2
0.4
0.6
0.8
1
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}

Dependence on Adhesive Stiffness



Tangential contact model



***Sliding* contact points:**

- static Coulomb friction

- dynamic Coulomb friction

- objectivity

Sliding/Rolling/Torsion

$$v_{\mathrm{t}} = \begin{cases} \left(v_i - v_j\right)^{\mathrm{t}} + \hat{n} \times \left(a_i \omega_i + a_j \omega_j\right) & \text{sliding} \\ a_{ij} \hat{n} \times \left(\omega_i - \omega_j\right) & \text{rolling} \\ a_{ij} \hat{n} \hat{n} \cdot \left(\omega_i - \omega_j\right) & \text{torsion} \end{cases}$$

Tangential contact model

- Static friction
- Dynamic friction

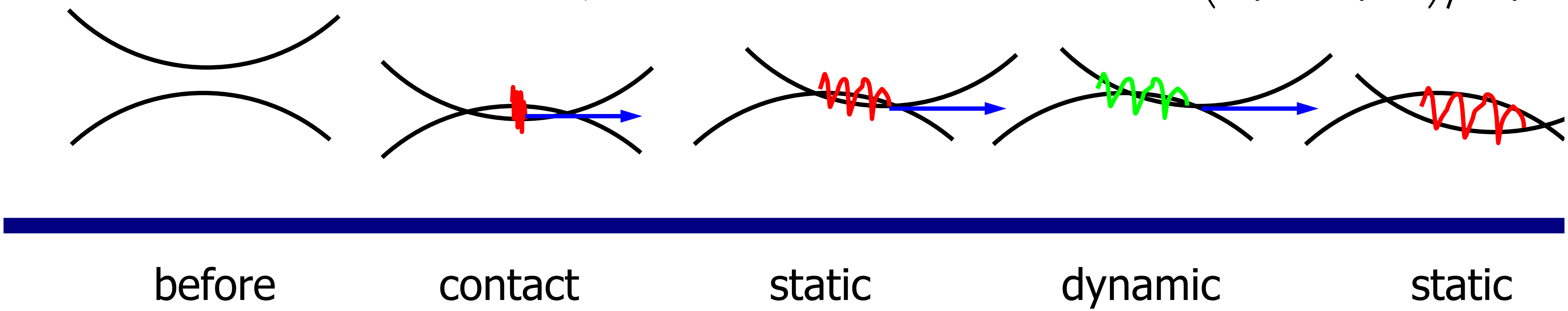
- spring
- dashpot

project into tangential plane $\vartheta' = \vartheta - \hat{n}\left(\hat{n} \cdot \vartheta\right)$

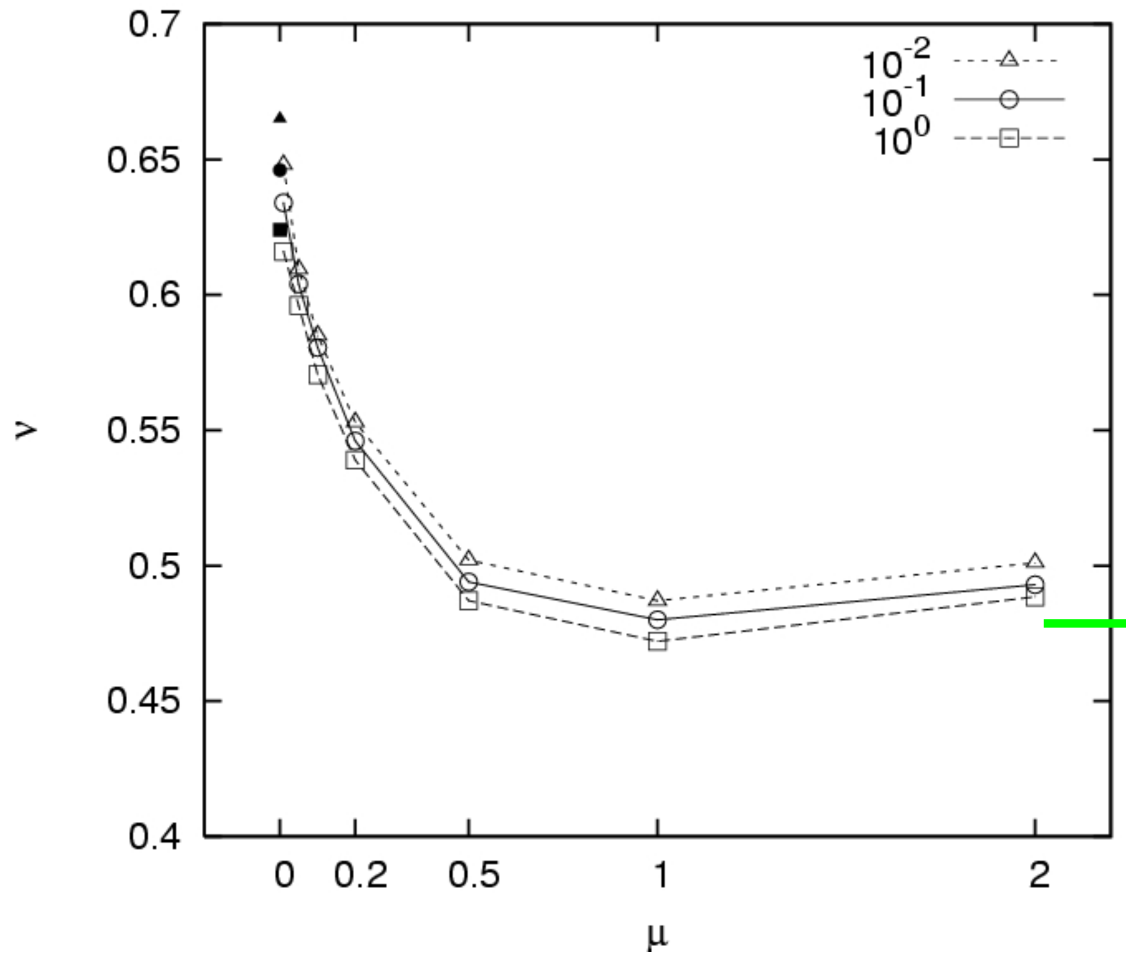
compute test force $f_\mathrm{t}^0 = -k_\mathrm{t}\vartheta' - \gamma_\mathrm{t}\dot{\vartheta}'$ and $\hat{t} = f_\mathrm{t}^0 \big/ \left|f_\mathrm{t}^0\right|$

sticking: $f_\mathrm{t}^0 \le \mu_\mathrm{s} f_\mathrm{n}$ $\quad f_\mathrm{t} = f_\mathrm{t}^0$ $\quad \vartheta = \vartheta' + \dot{\vartheta}'\,\mathrm{d}t$

sliding: $f_\mathrm{t}^0 > \mu_\mathrm{s|d} f_\mathrm{n}$ $\quad f_\mathrm{t} = \mu_\mathrm{d} f_\mathrm{n}\,\hat{t}$ $\quad \vartheta = \left(f_\mathrm{t} + \gamma_\mathrm{t}\dot{\vartheta}'\right)\big/ k_\mathrm{t}$



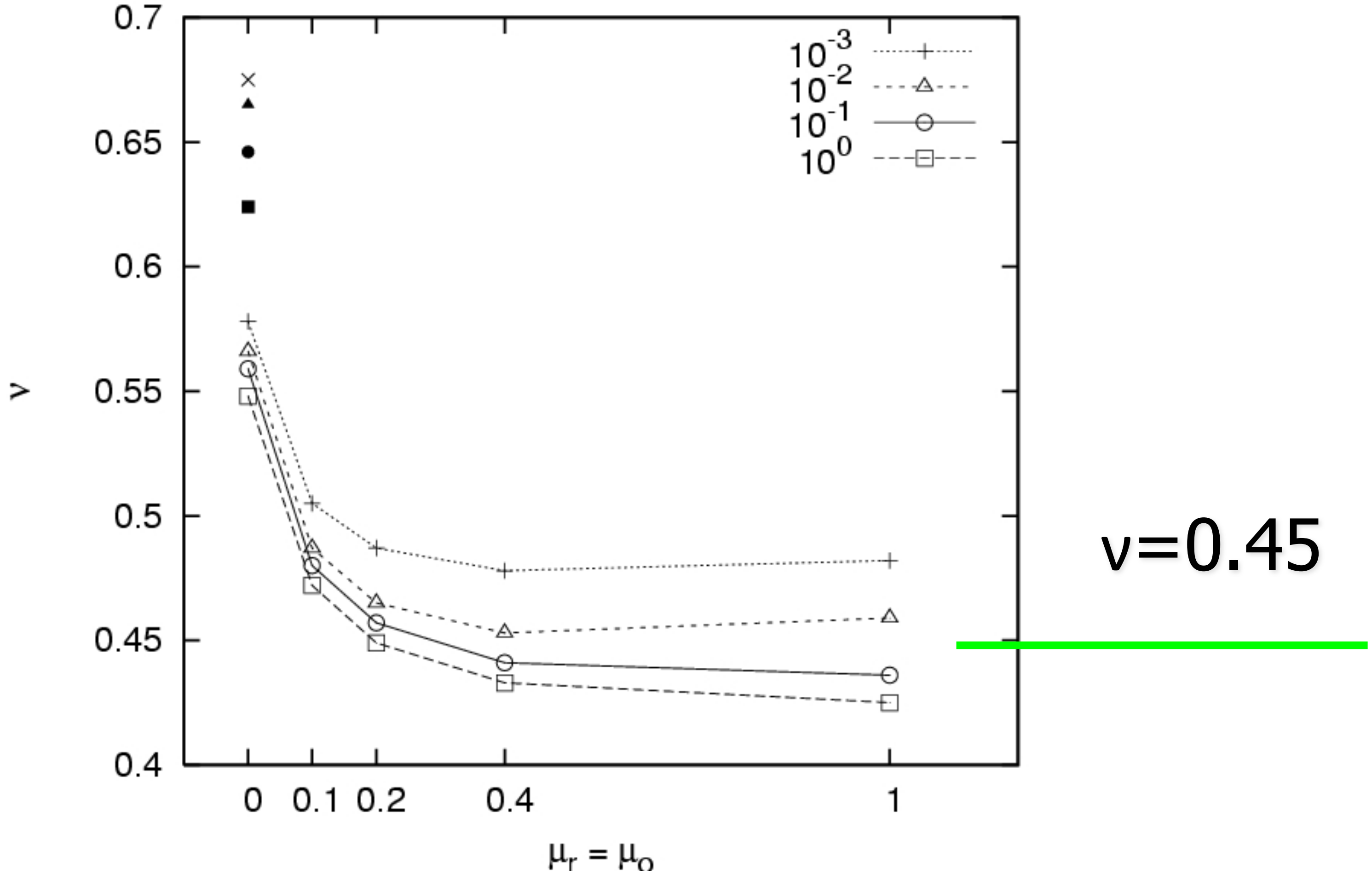
3D – Density vs. friction …



ν=0.48

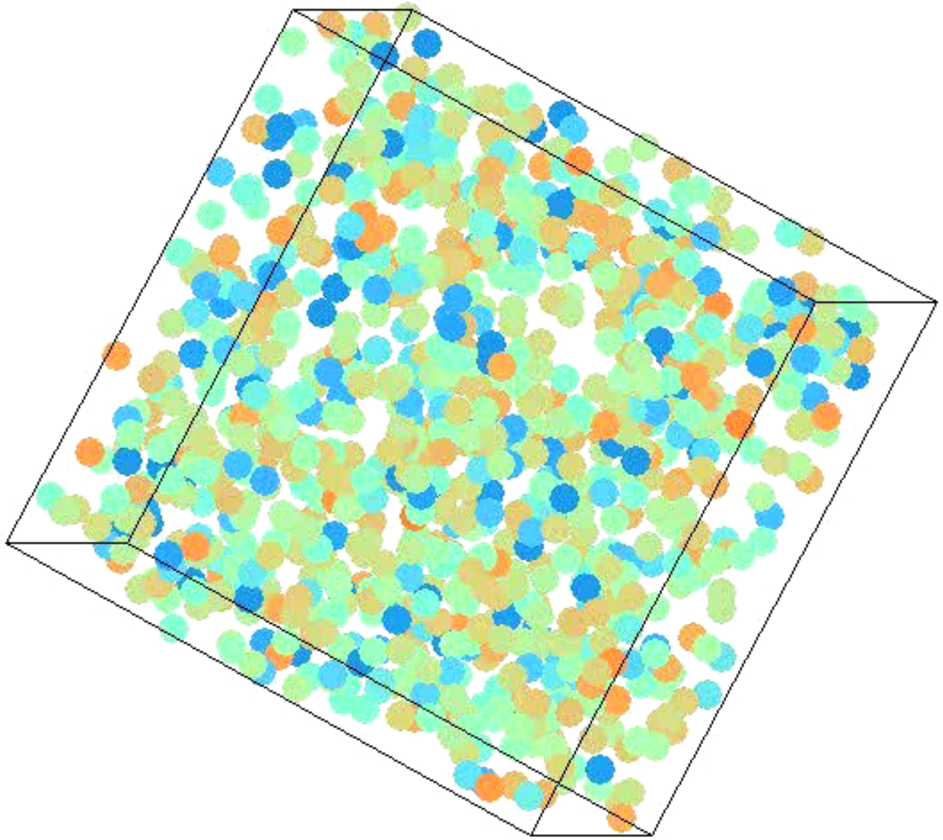
- Saturation at strong friction

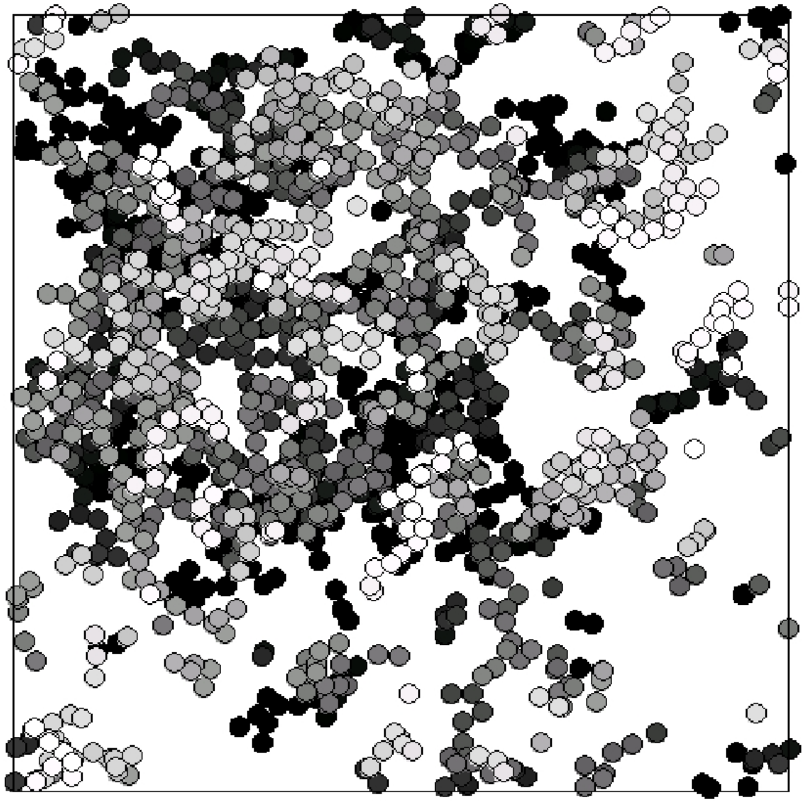
3D – Density vs. rolling-resistance



- Saturation at high rolling resistance

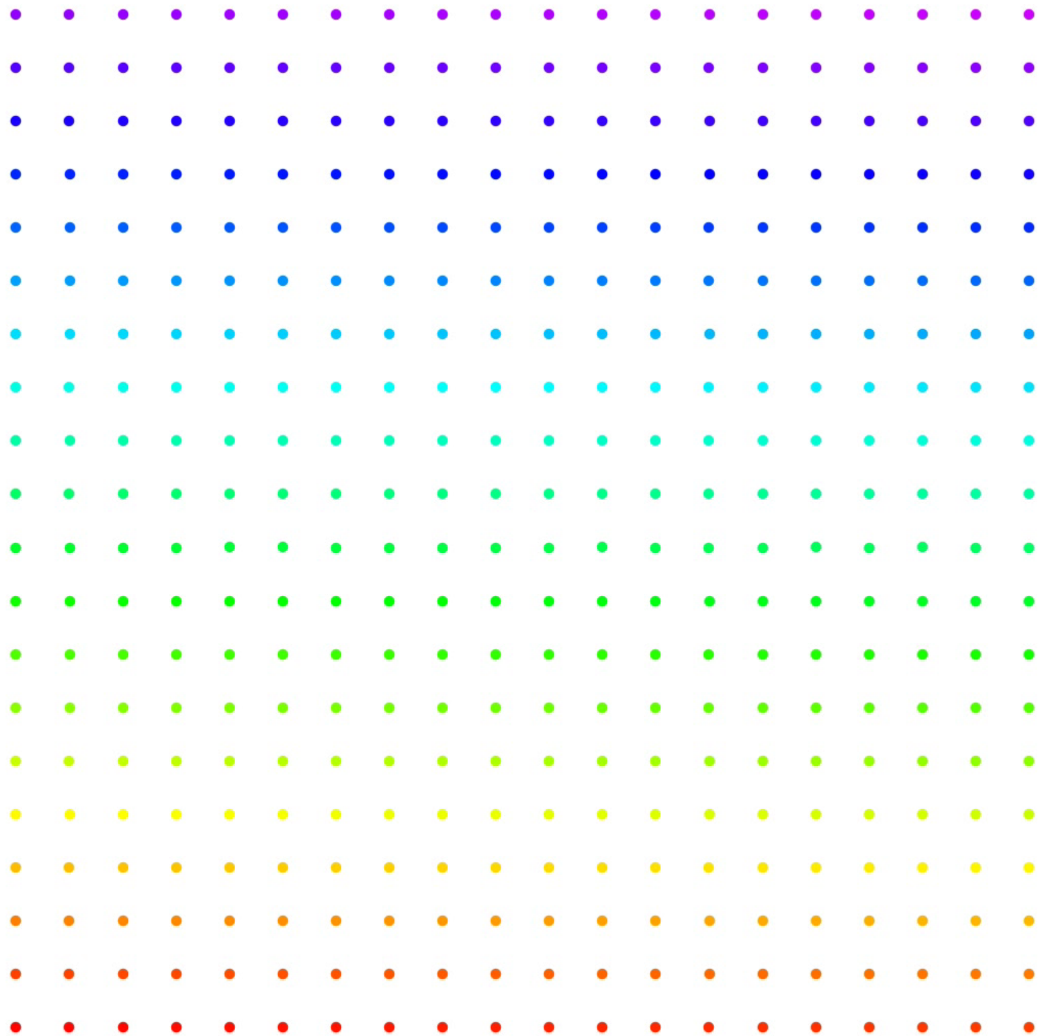
… details of interaction





Attraction + Dissipation = Agglomeration

Example: Agglomeration



S. Gonzalez-Briones, MSM, 2010

Challenge

- Particle *Agglomeration/Clustering*
  - *1) Without longrange forces*
  - *2) With longrange forces*

GAS

↓

FLUID

↓

SOLID

We can simulate:

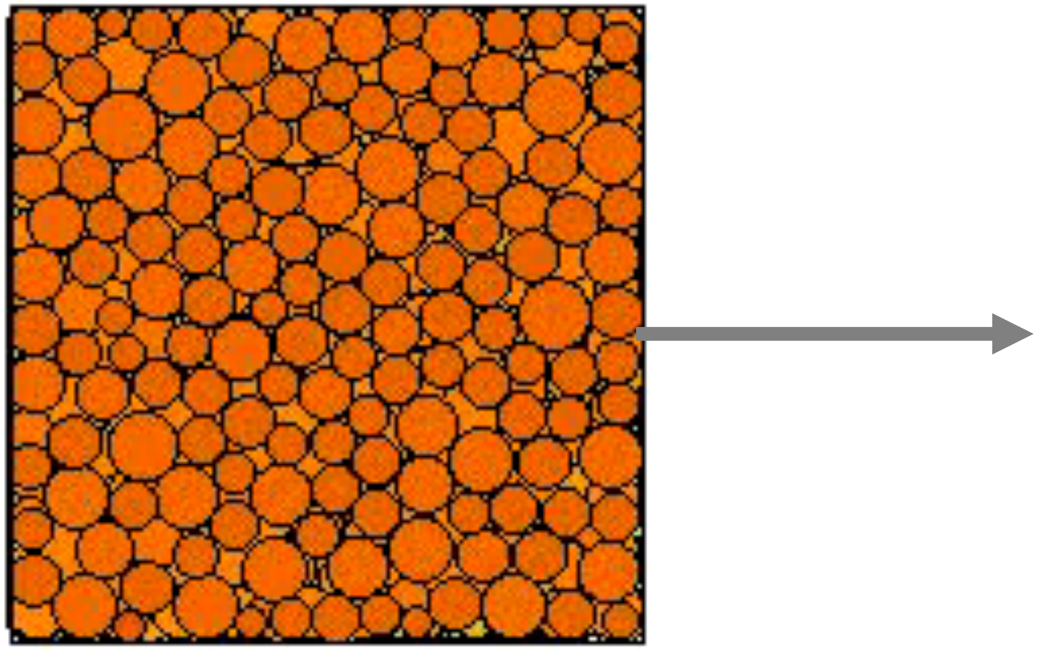
+ element tests (REV)
+ small processes & equipment

– large scales (processes/plants/geophysical scales)
– especially of fine, cohesive powders

Instead:
+ provide constitutive relations = f(contact)
+ model large scales with continuum methods

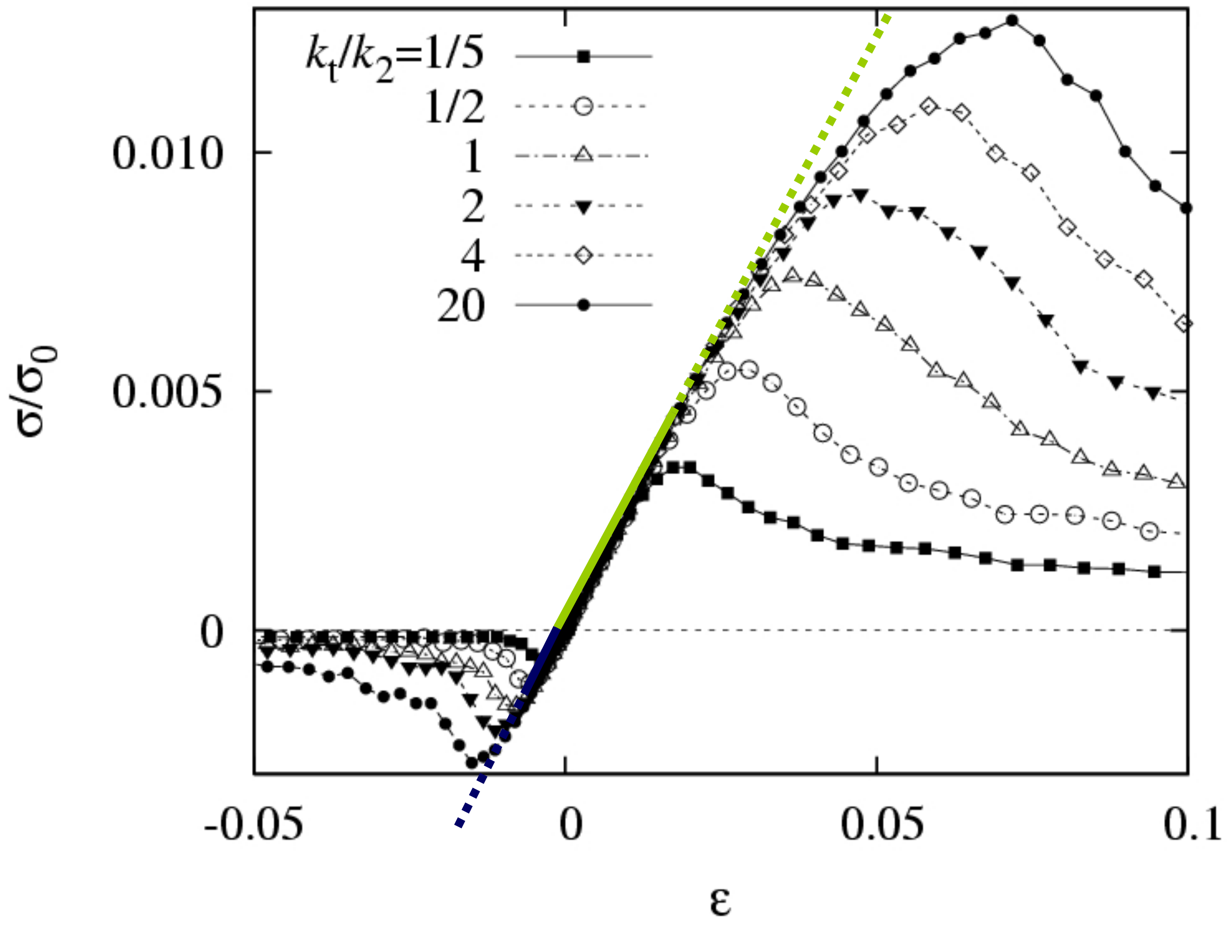
tension - uni-axial

$k_t / k_2 = 1/2$



uni-axial compression-tension

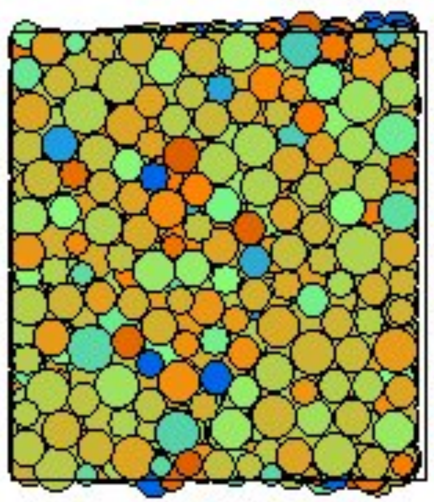
- Compression
- Tension

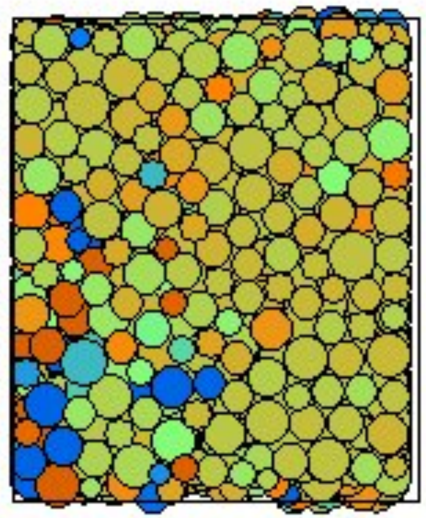


compression - uni-axial

$$k_t / k_2 = 1/2$$

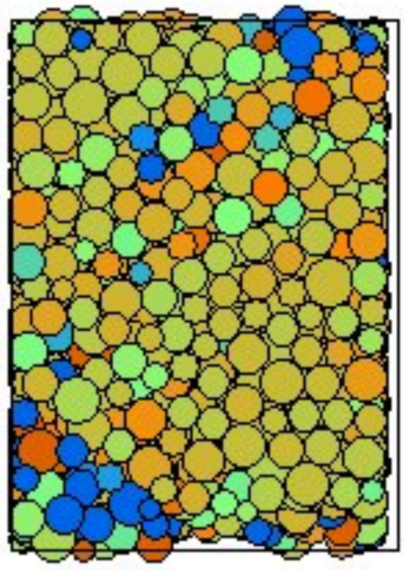
compression - uni-axial

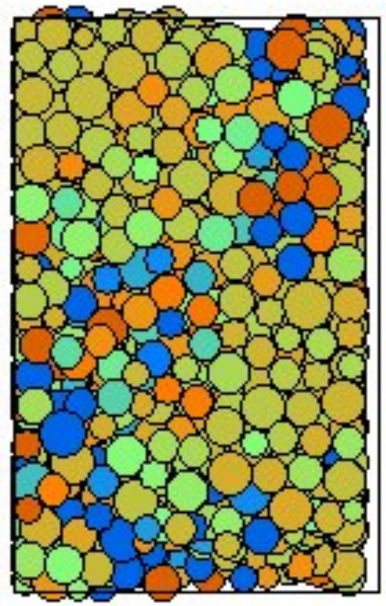




$$k_t / k_2 = 1/2$$

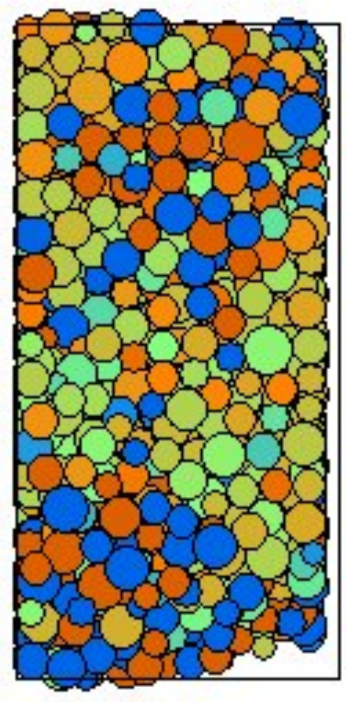
compression - uni-axial

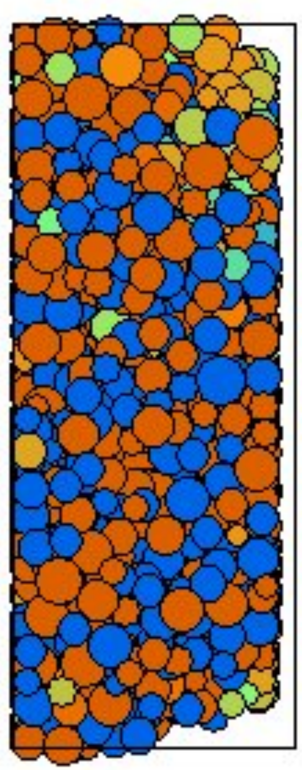




$k_t / k_2 = 1/2$

compression - uni-axial

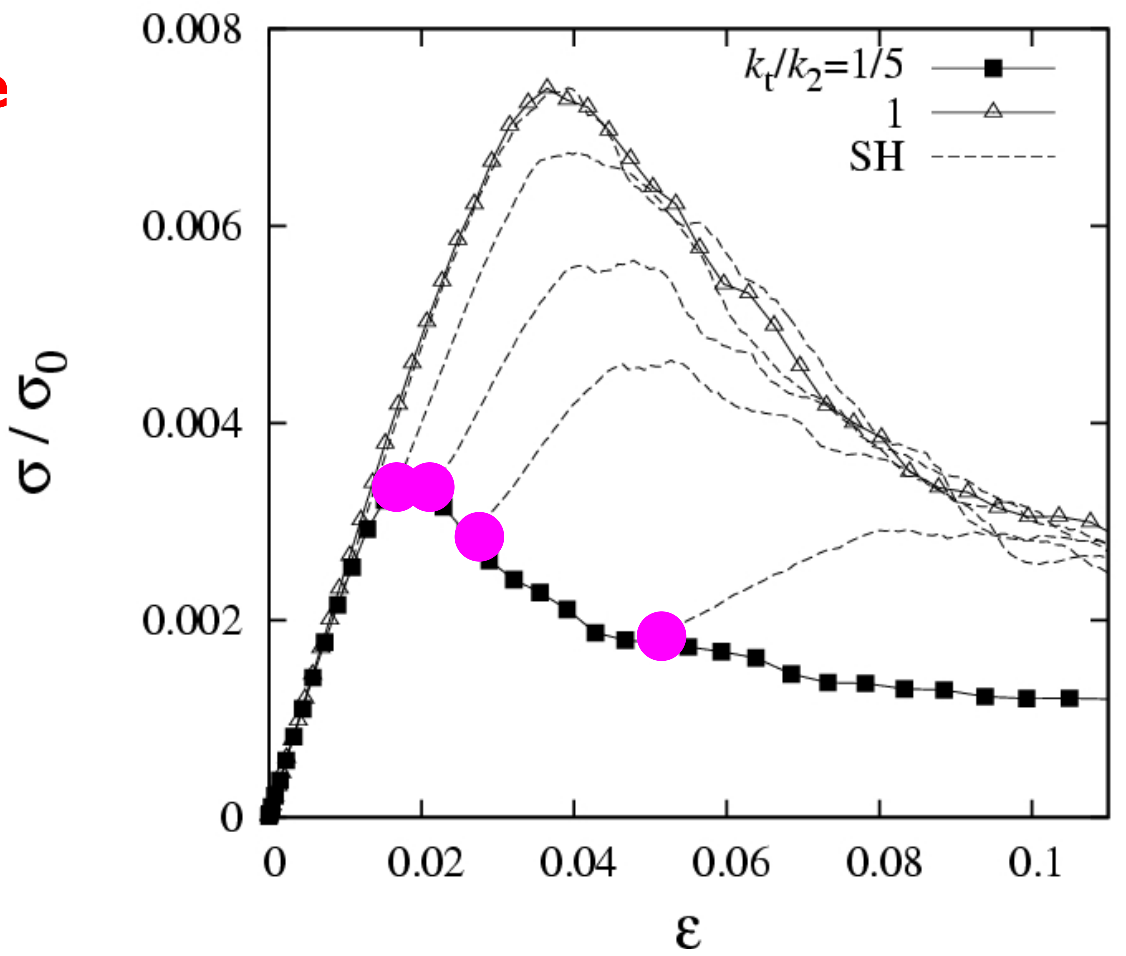




$$k_t / k_2 = 1/2$$

healing (compression)

1. Preparation
2. HIGH pressure
3. Relaxation
4. Compression
5. Tension
6. Healing



Overview

Introduction

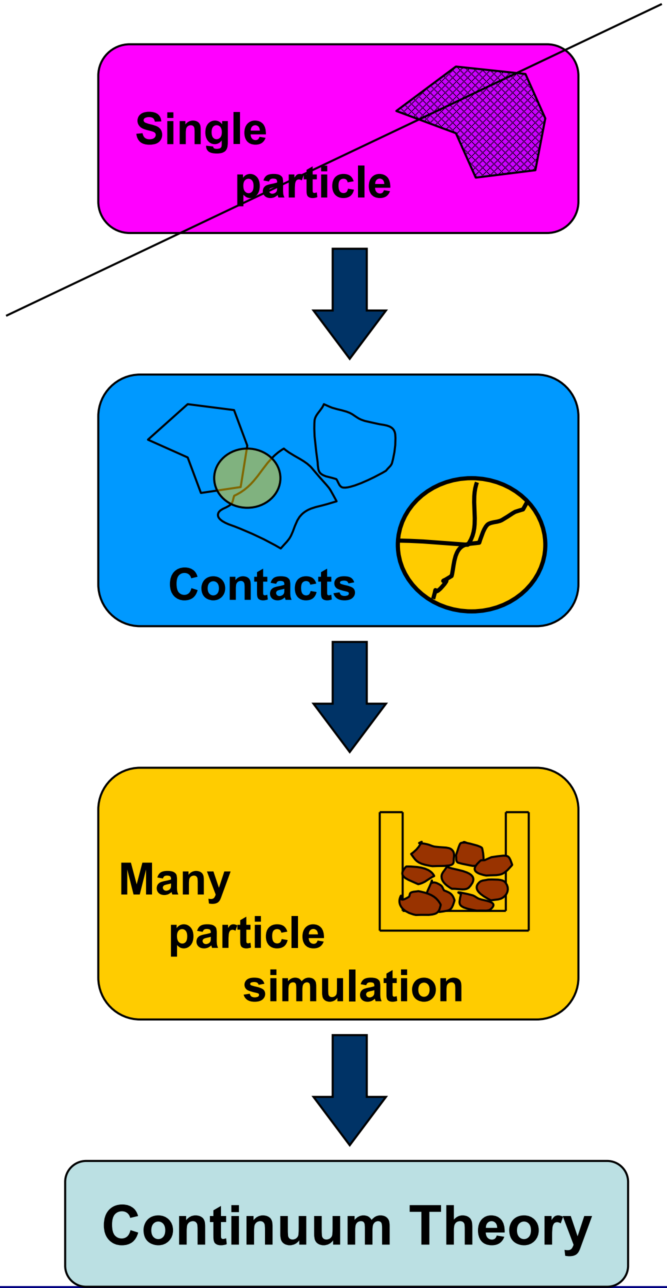
Meso-contact **models**

MESO particle simulation

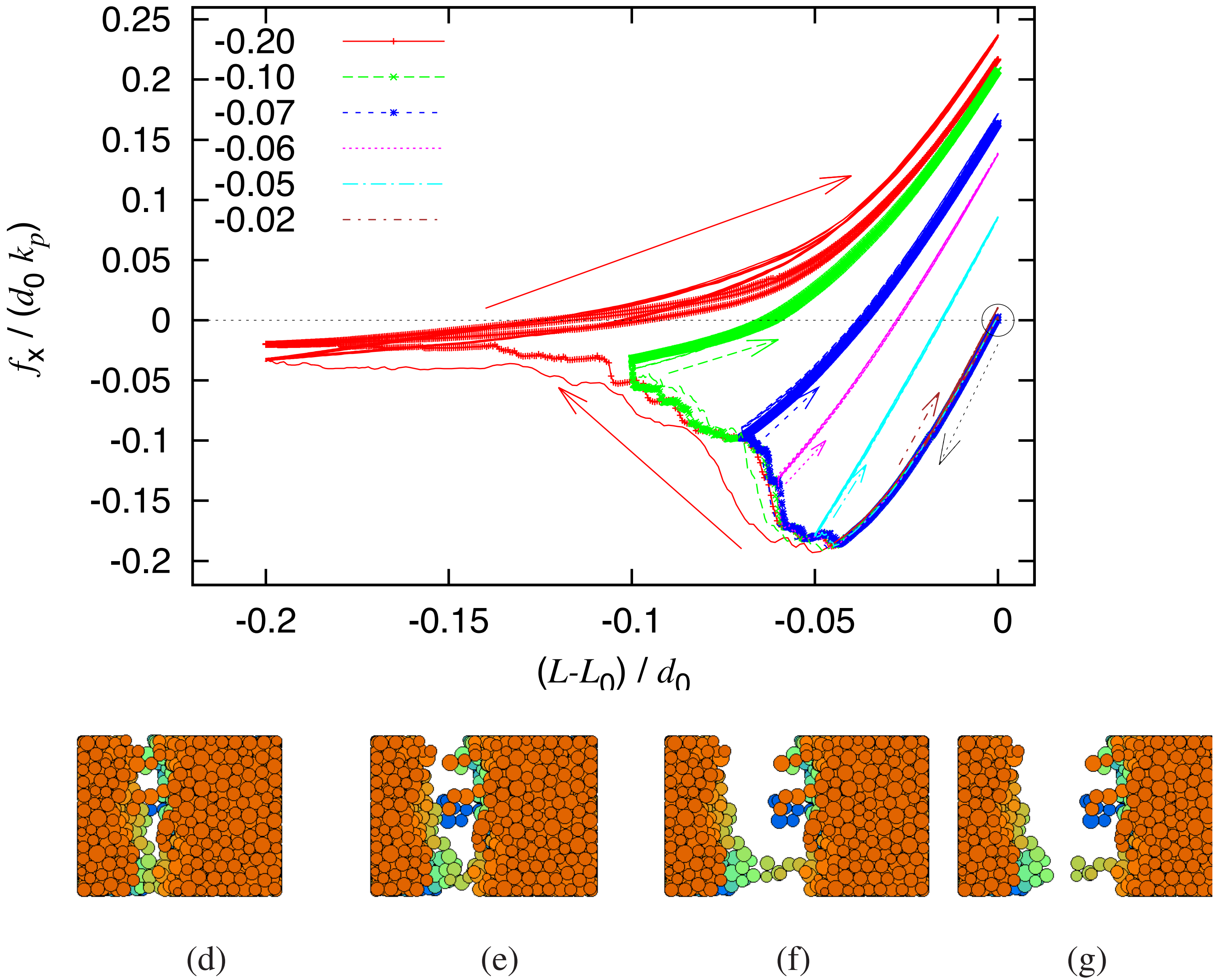
Global/Local micro-macro

Continuum Theory

… with microstructure

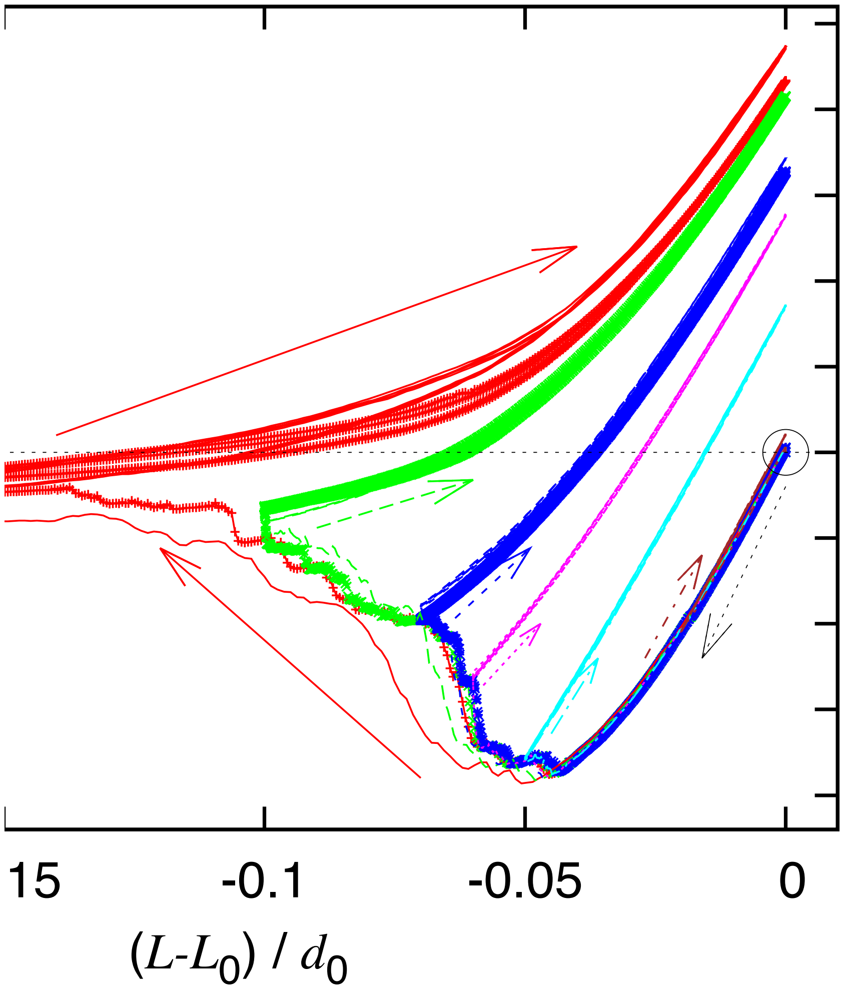


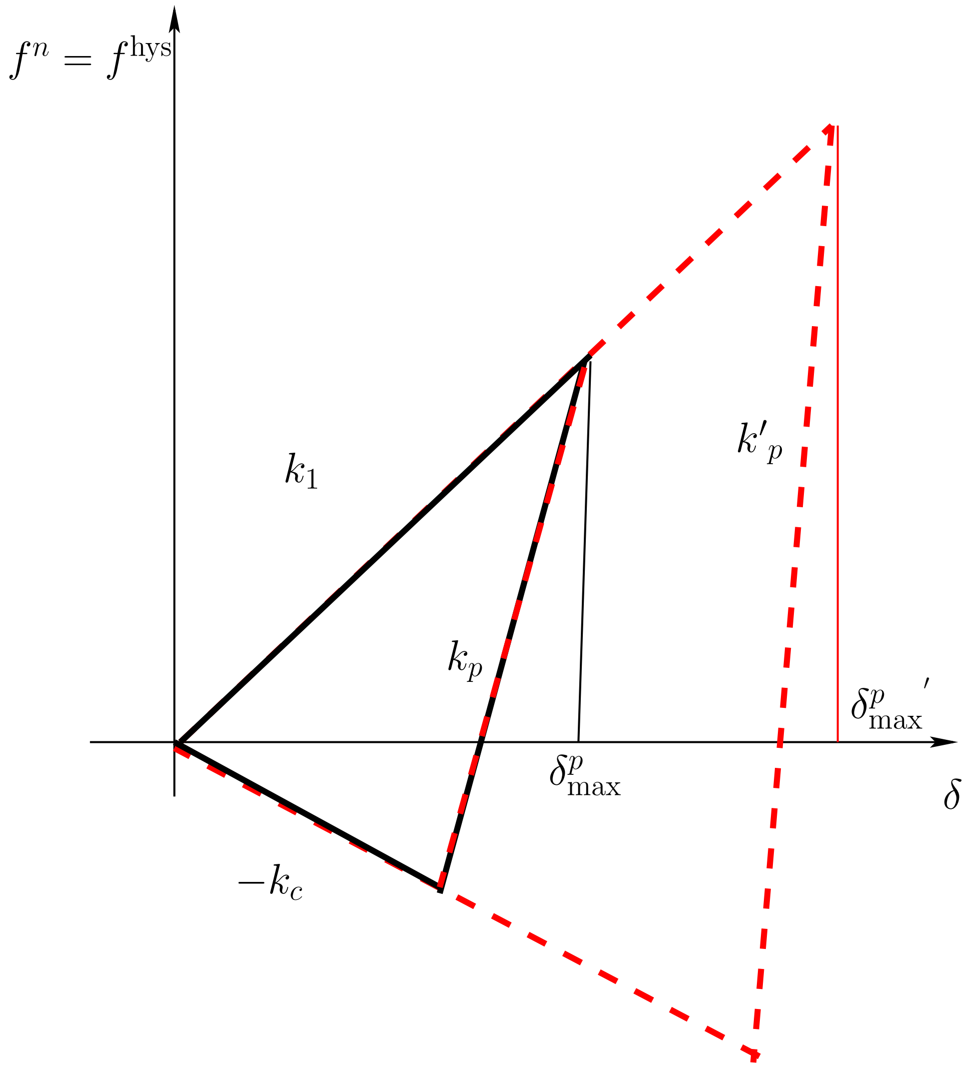
Meso



Meso = superposition of many primary p.

Meso contacts ...





Meso = superposition of many primary p.

Meso contacts …
+ coarse = up-scaled particles

represent many primary particles

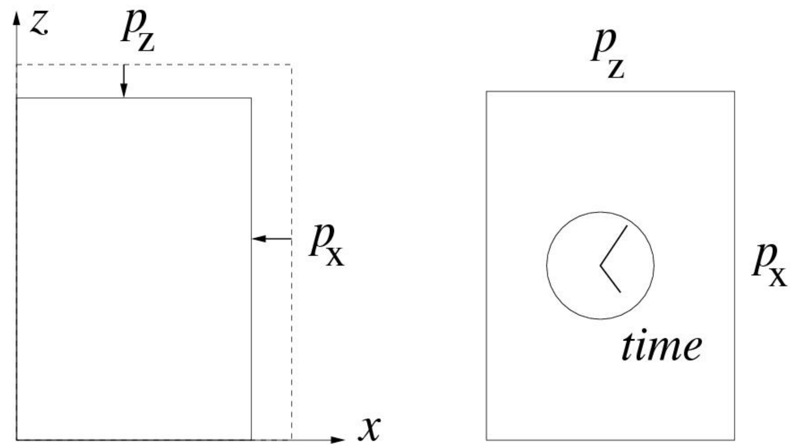
one way of multi-scale modeling

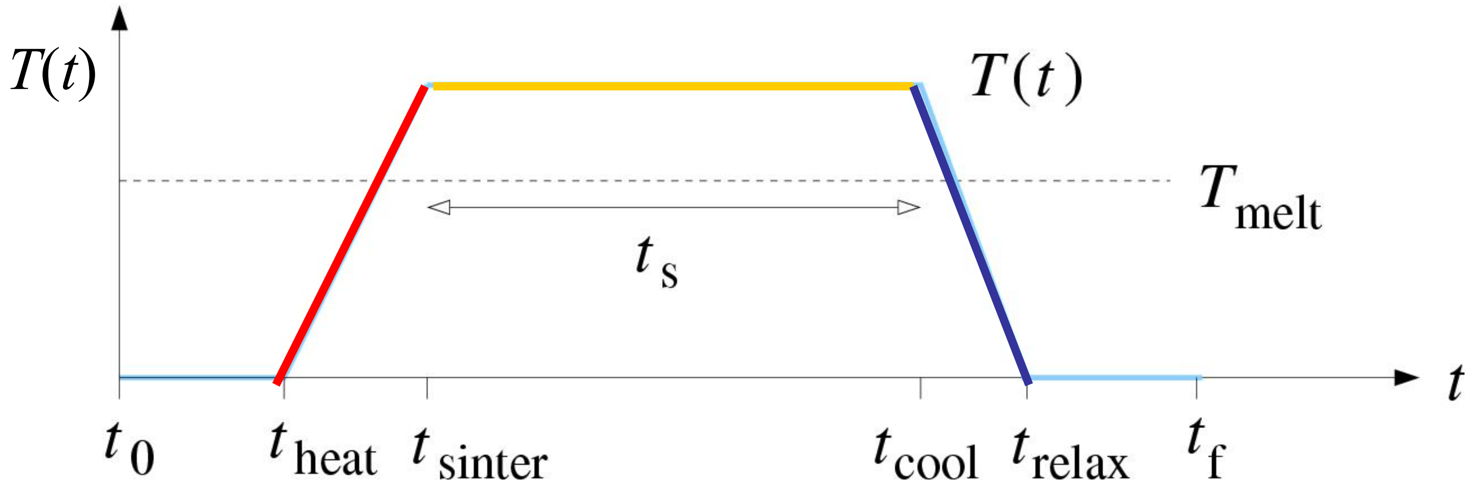
attention: does not always work!

Meso = superposition of many primary p.

Sintering / Cementation (back to 2D)

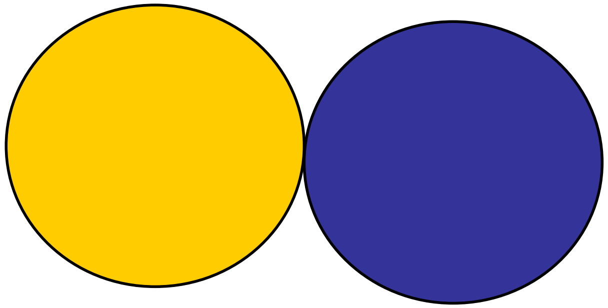
1. Preparation
2. Heating
3. Sintering / Cementation
4. Cooling
5. Relaxation
6. Testing



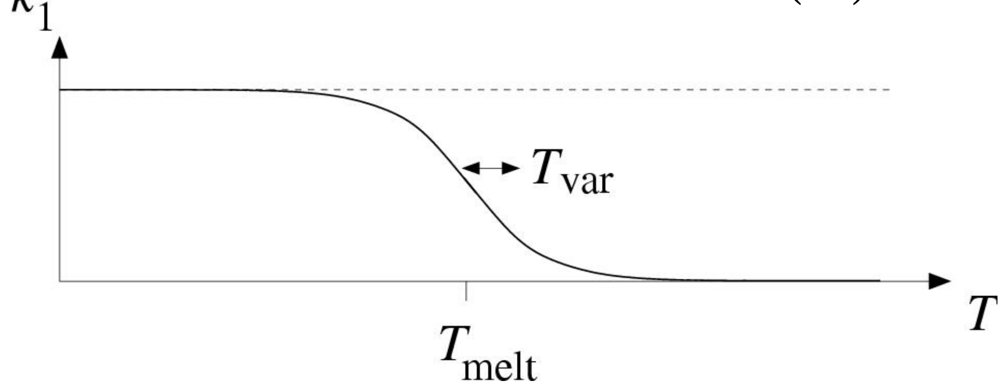


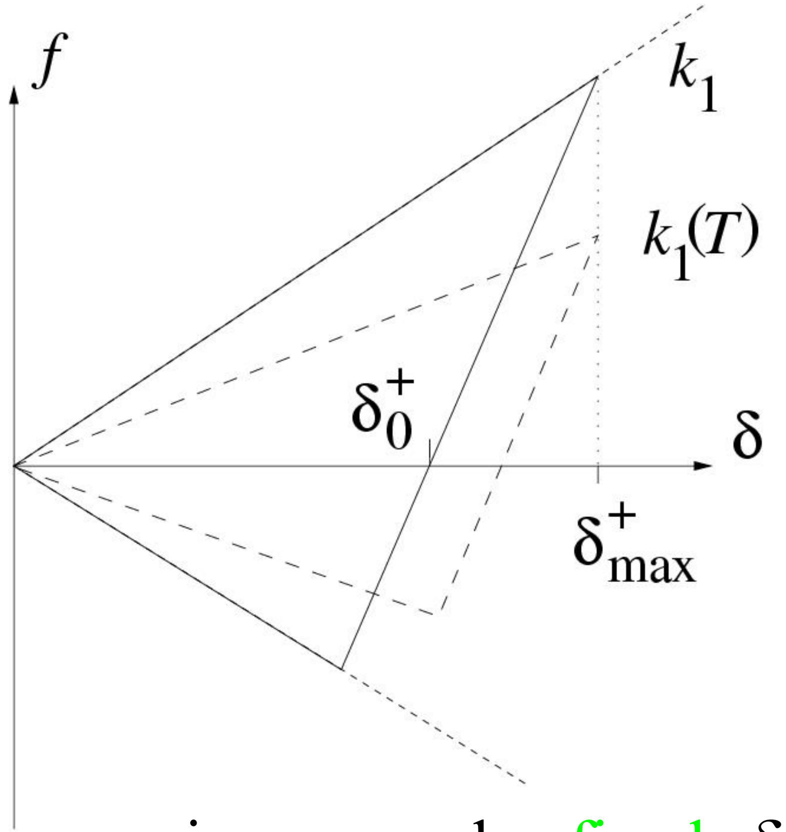
Sintering / Cementation 2

2. Heating



loading stiffness: $k_1 = k_1(T)$



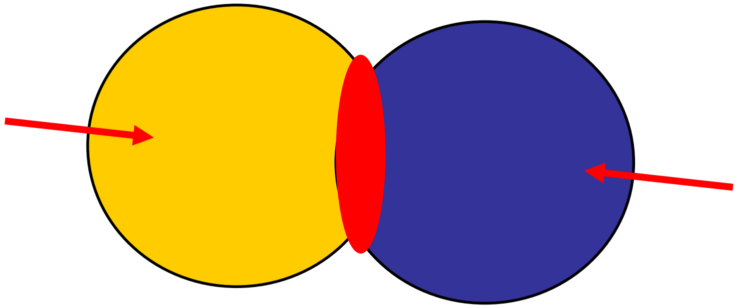


maximum overlap fixed: δ_{max}^+

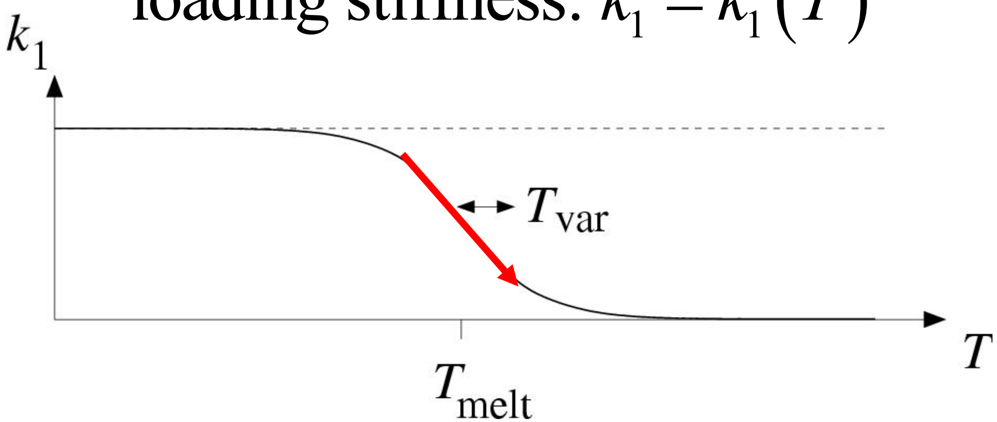
neutral overlap increasing: δ_0^+

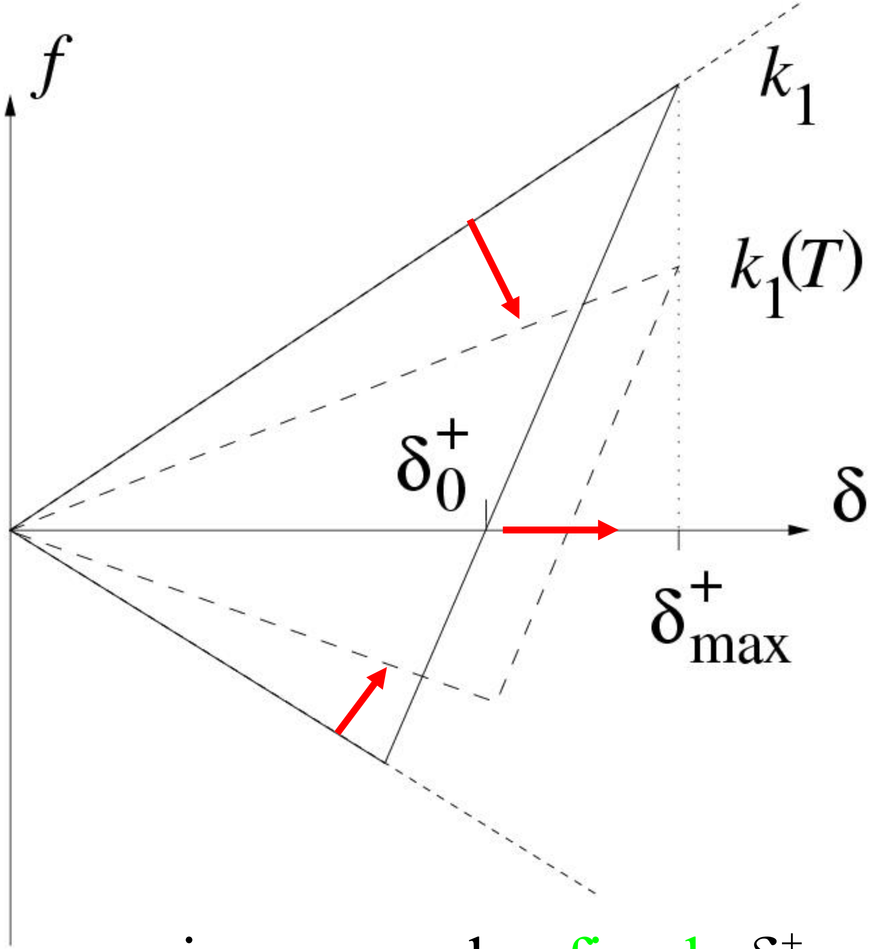
Sintering / Cem.

2. Heating



loading stiffness: $k_1 = k_1(T)$



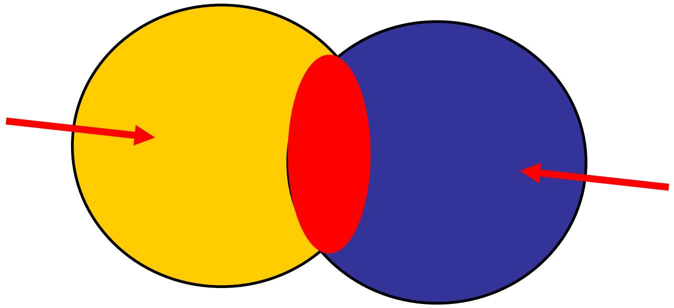


maximum overlap fixed: δ_{max}^+

neutral overlap increasing: δ_0^+

Sintering / Cem. 3

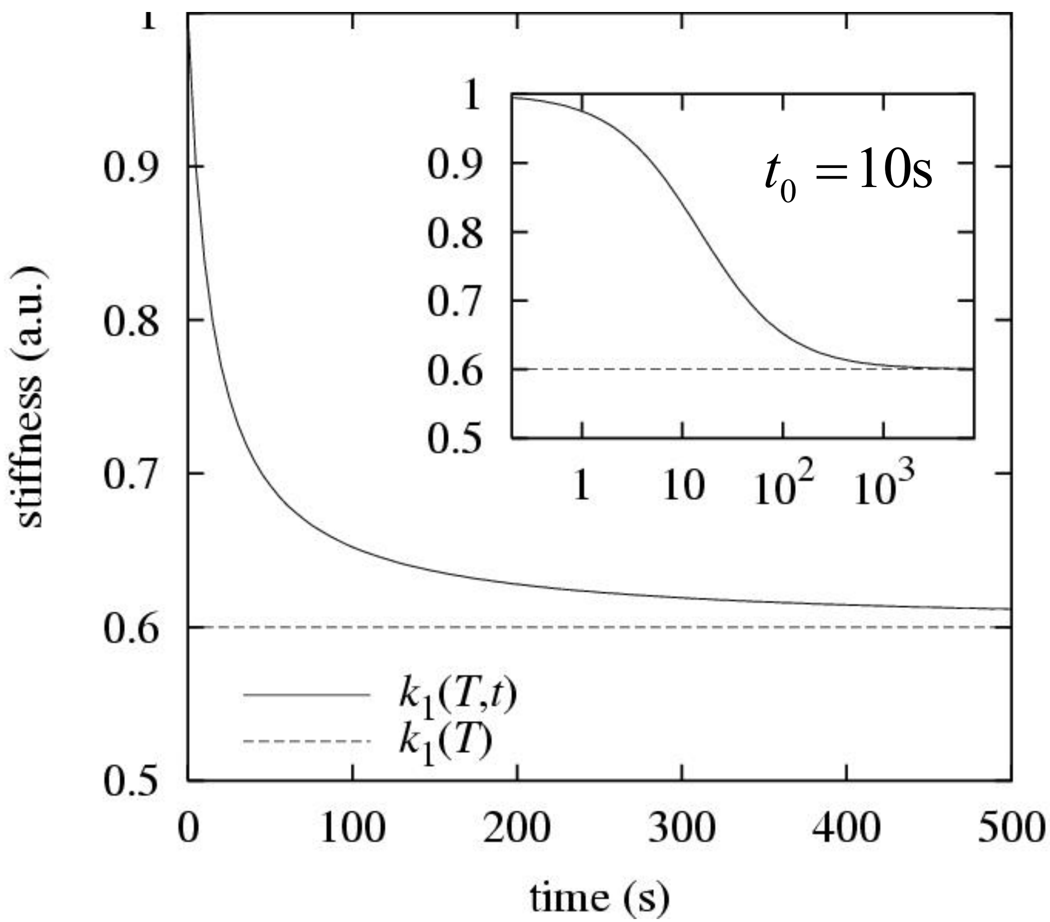
3. Sintering / Cementation - Reaction



Sintering 3

3. Sintering

- slow dynamics (t_0)
- diffusion, …
- trick: increase t_0

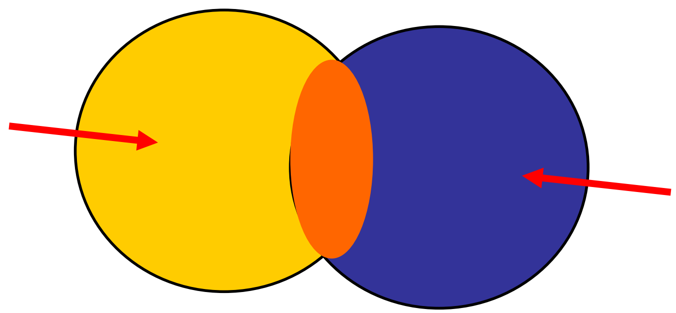


time delay:

$$\frac{\partial}{\partial t} k_1(T,t) = \pm \frac{\left[k_1(T) - k_1(T,t)\right]^2}{k_1(T)\, t_0} \qquad k_1(T,t) = k_1(T)\left\{1 - \left(\frac{1}{1 - k_1(T_0)/k_1(T)} - \frac{t}{t_0}\right)^{-1}\right\}$$

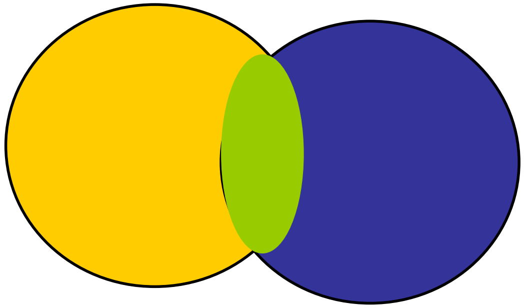
Sintering 4

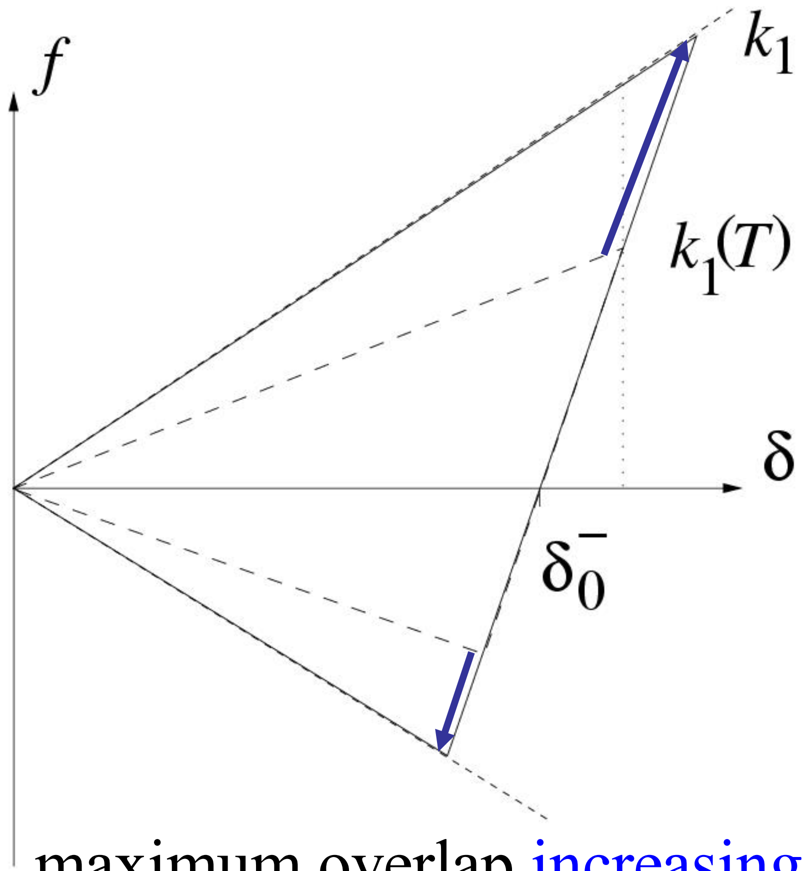
4. Cooling



Sintering 4

4. Cooling



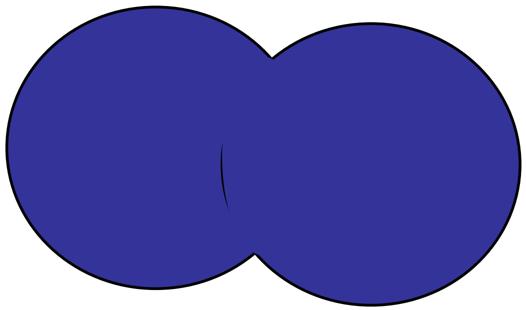


maximum overlap increasing: δ_{max}^-

neutral overlap fixed: δ_0^-

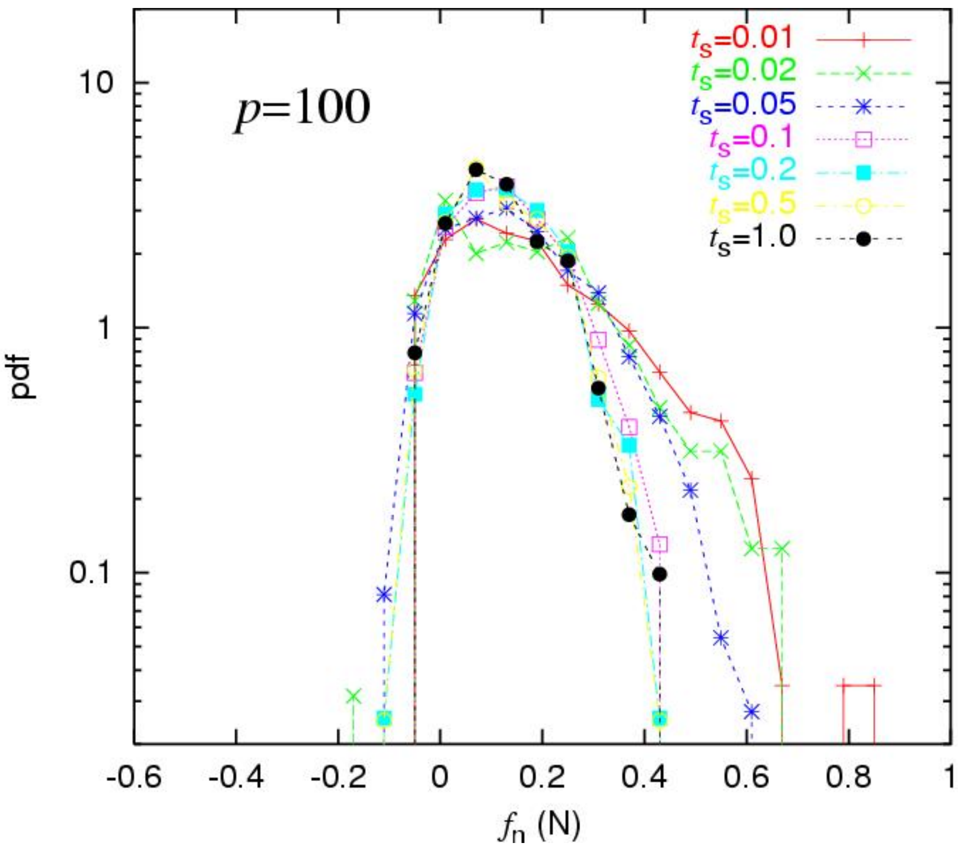
Sintering 5

5. Relaxation

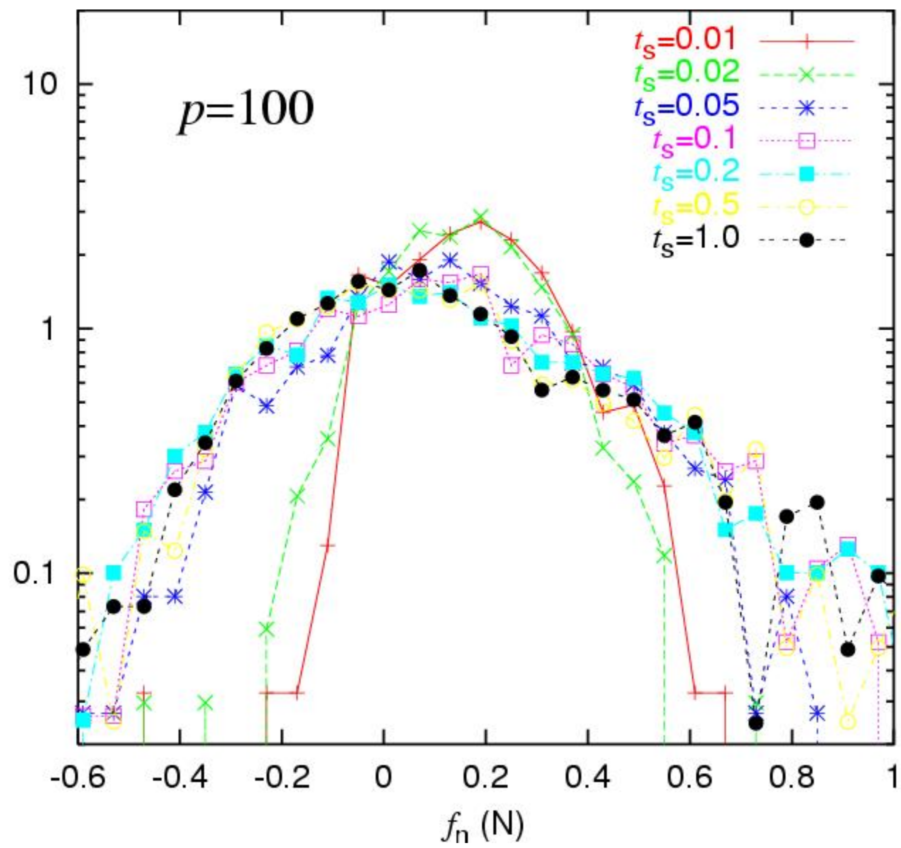


Contact forces

after Sintering

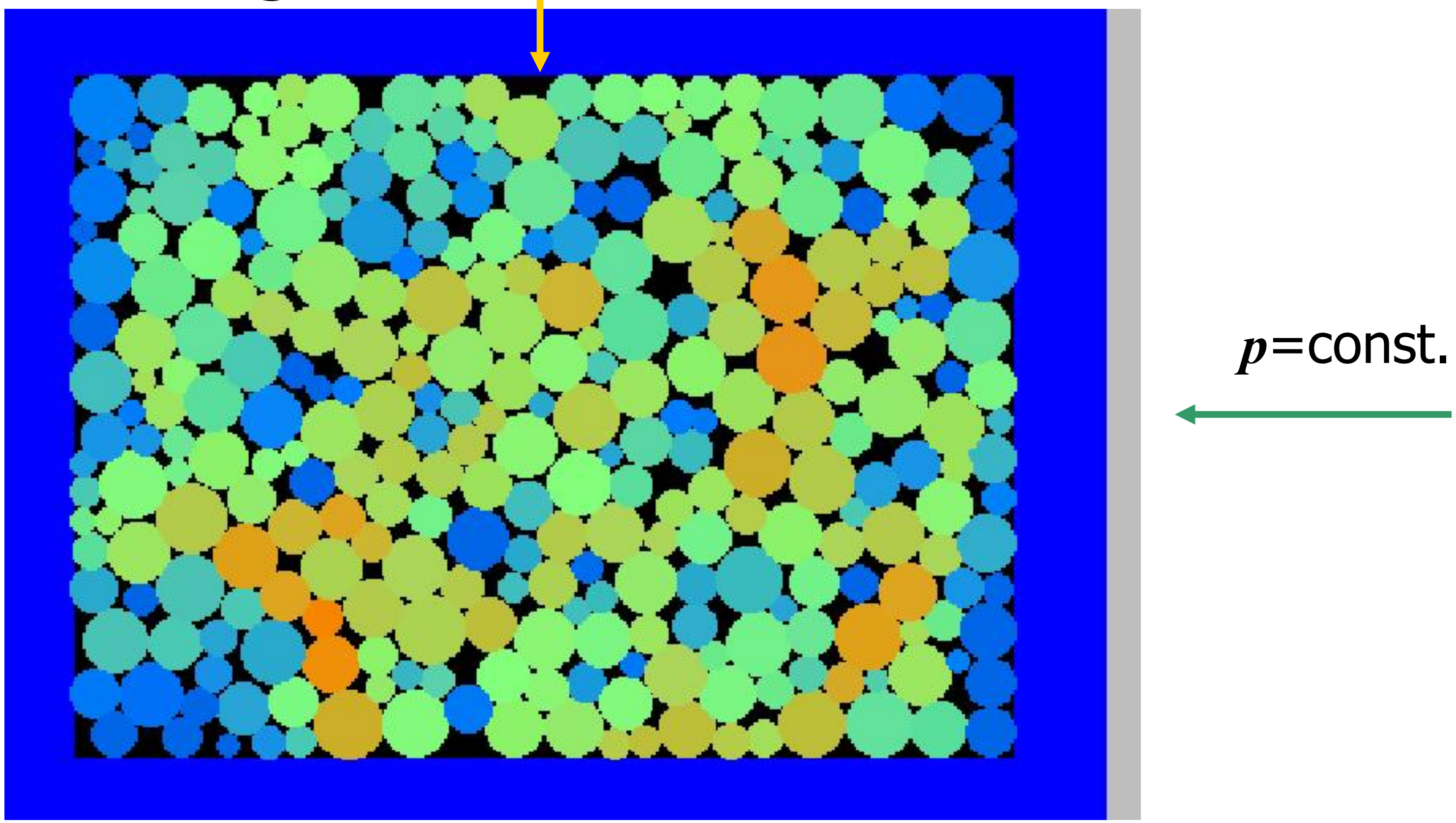


after Relaxation



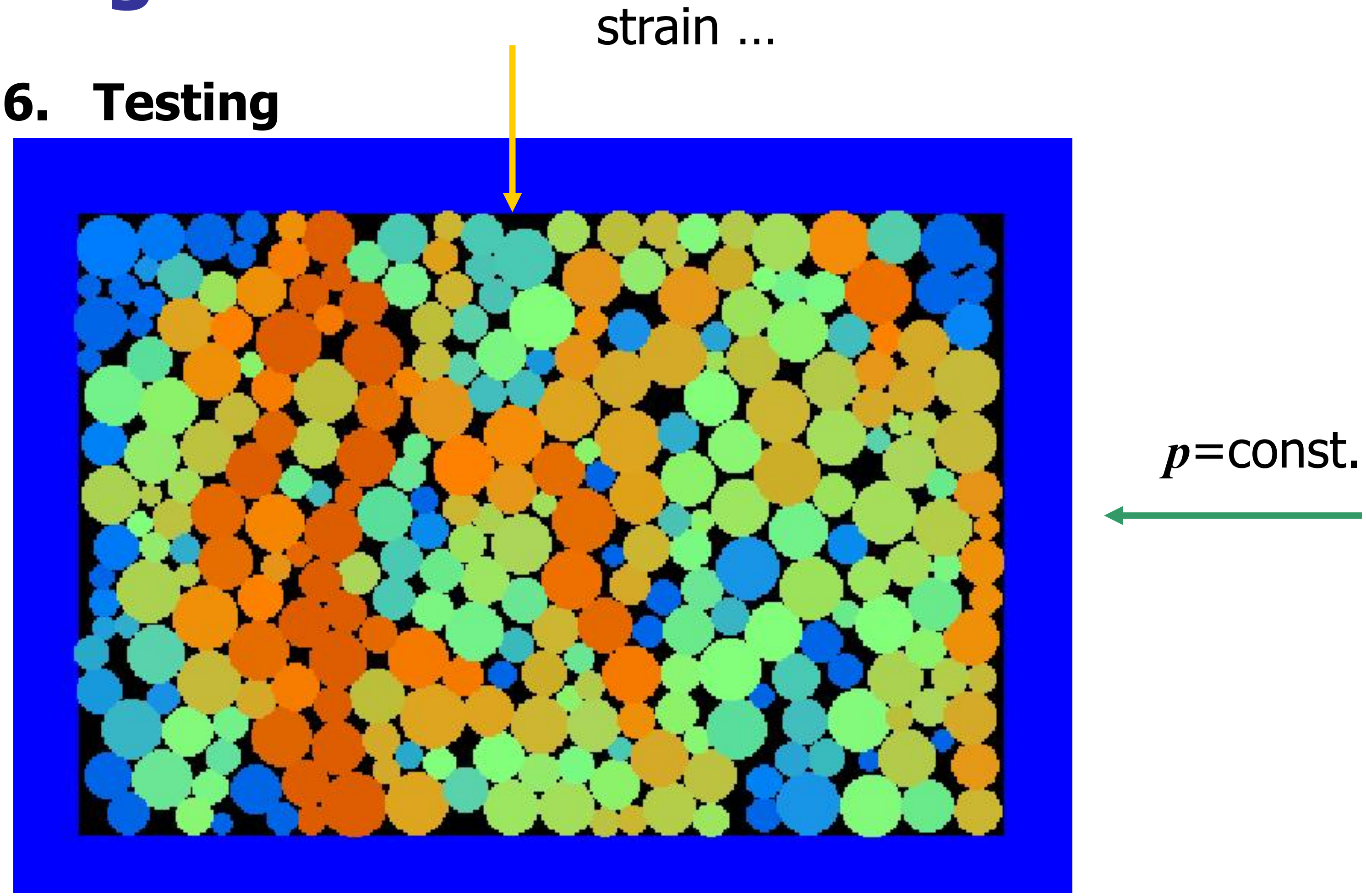
Sintering 6

6. Testing



Sintering 6

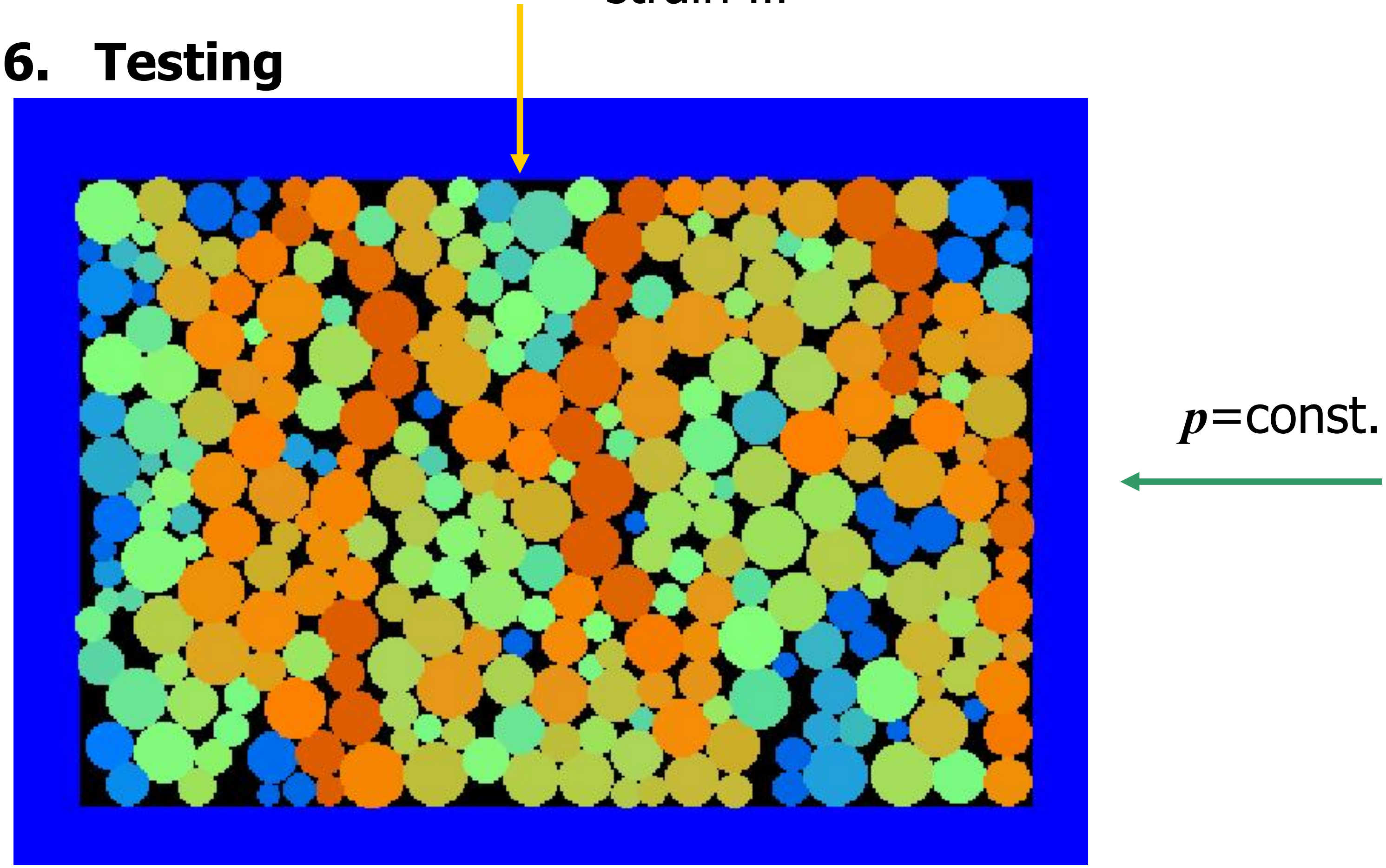
6. Testing



Sintering 6

strain ...

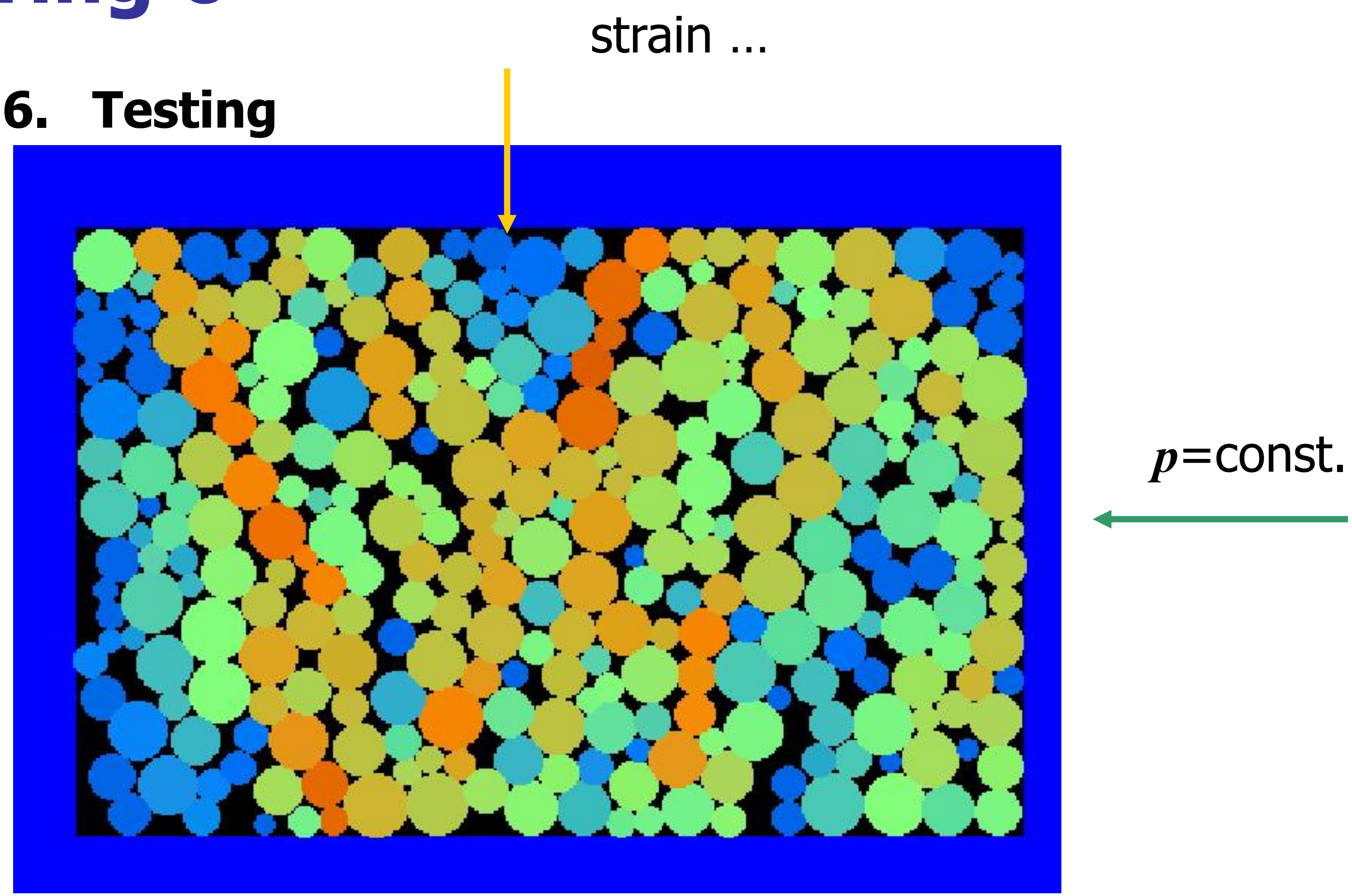
6. Testing



p=const.

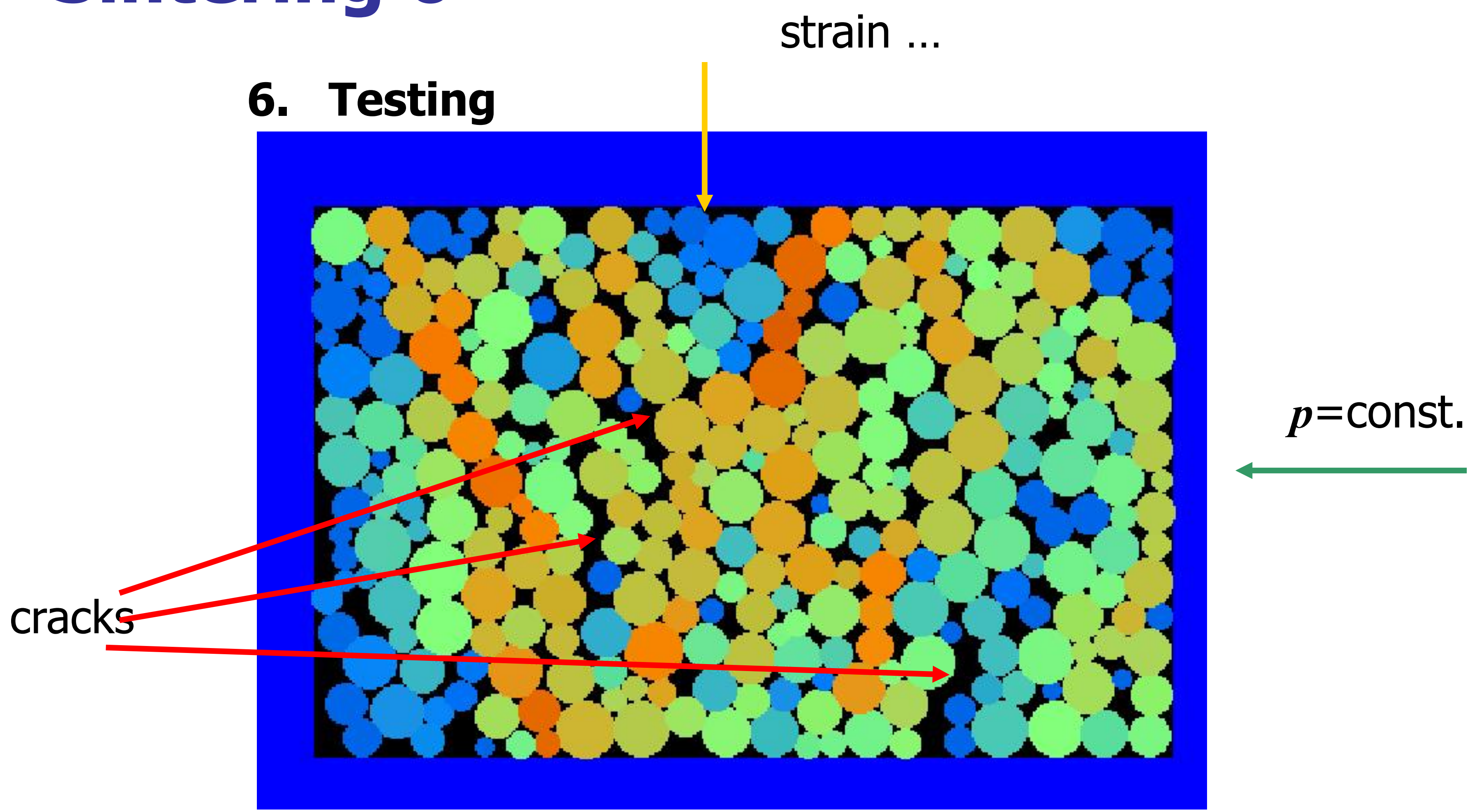
Sintering 6

6. Testing



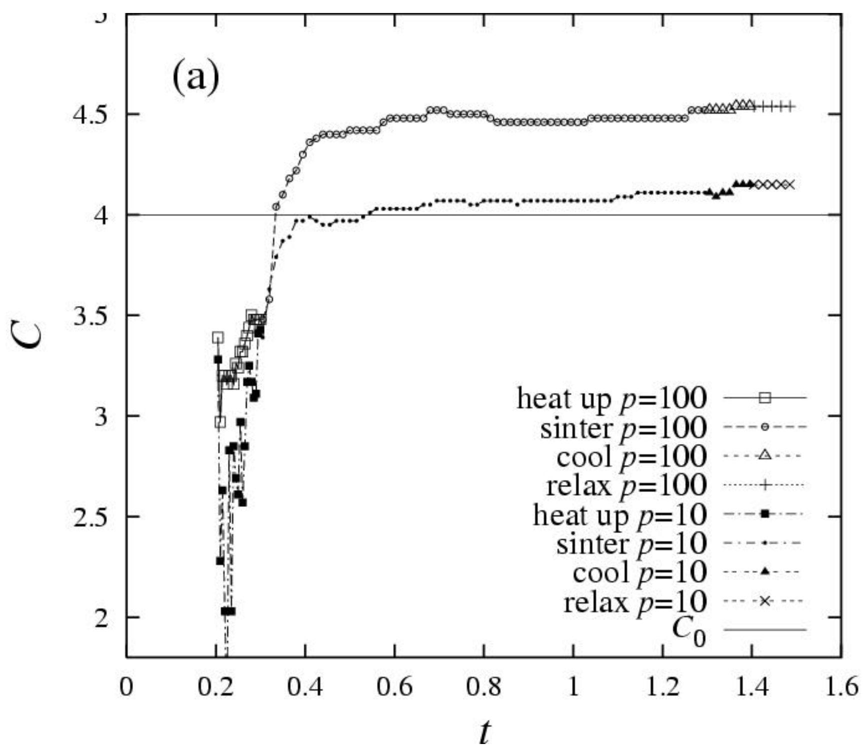
Sintering 6

6. Testing

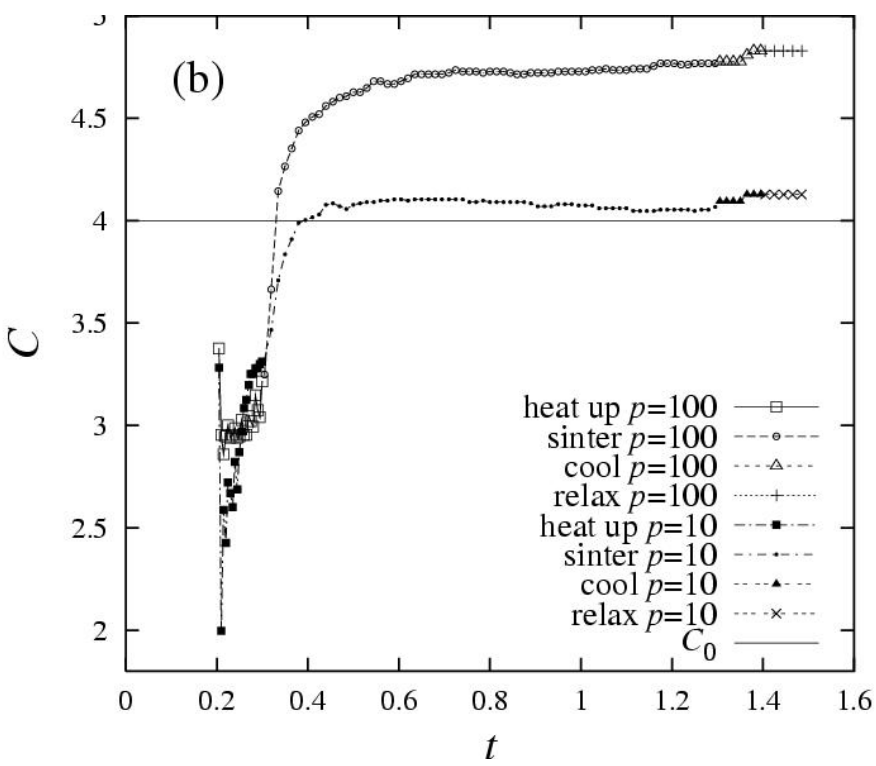


Sintering 6

Contact number



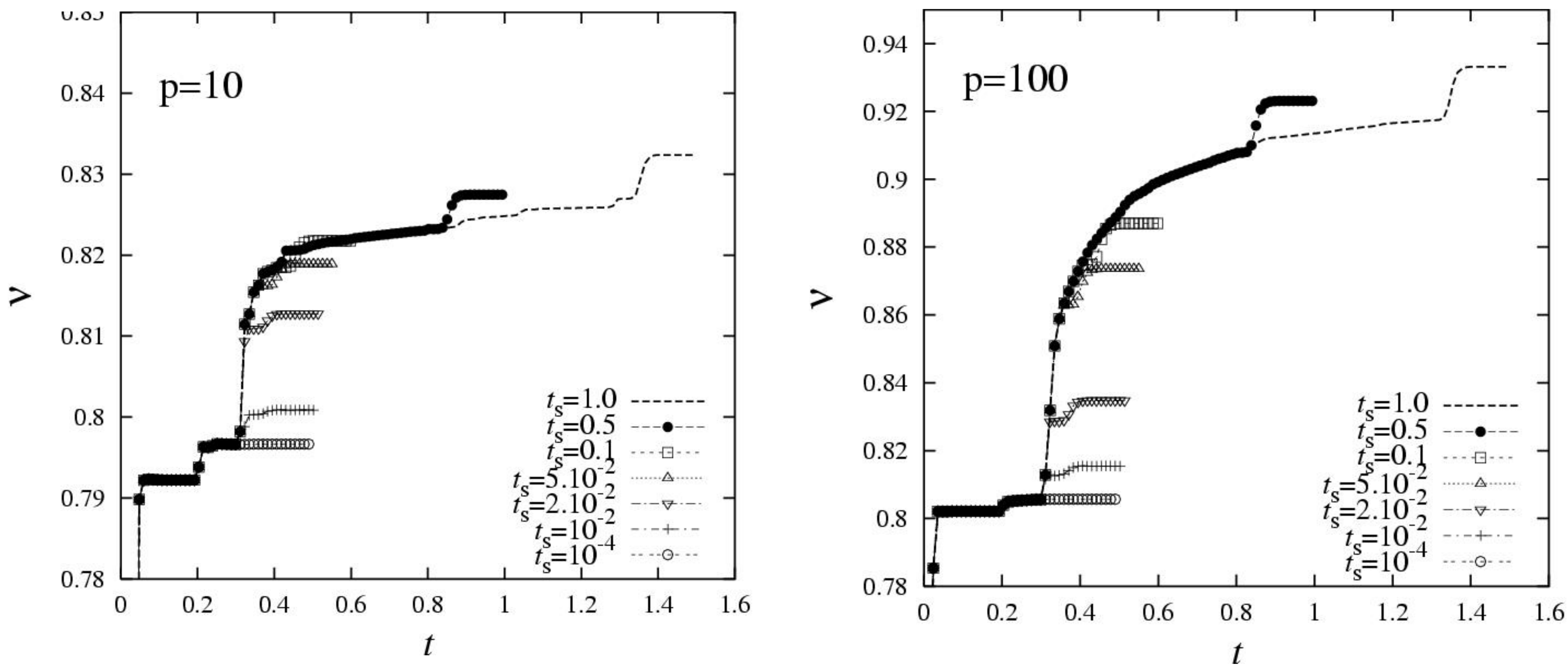
N=100



N=300

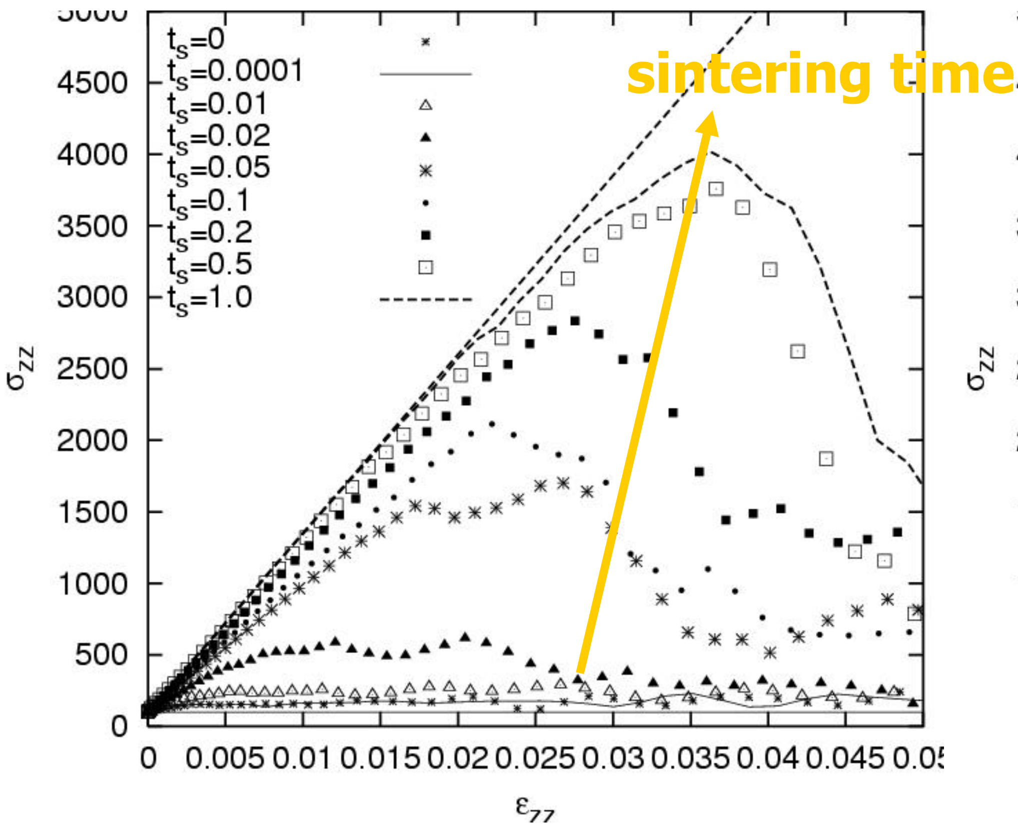
Sintering 6

Density – Shrinkage!

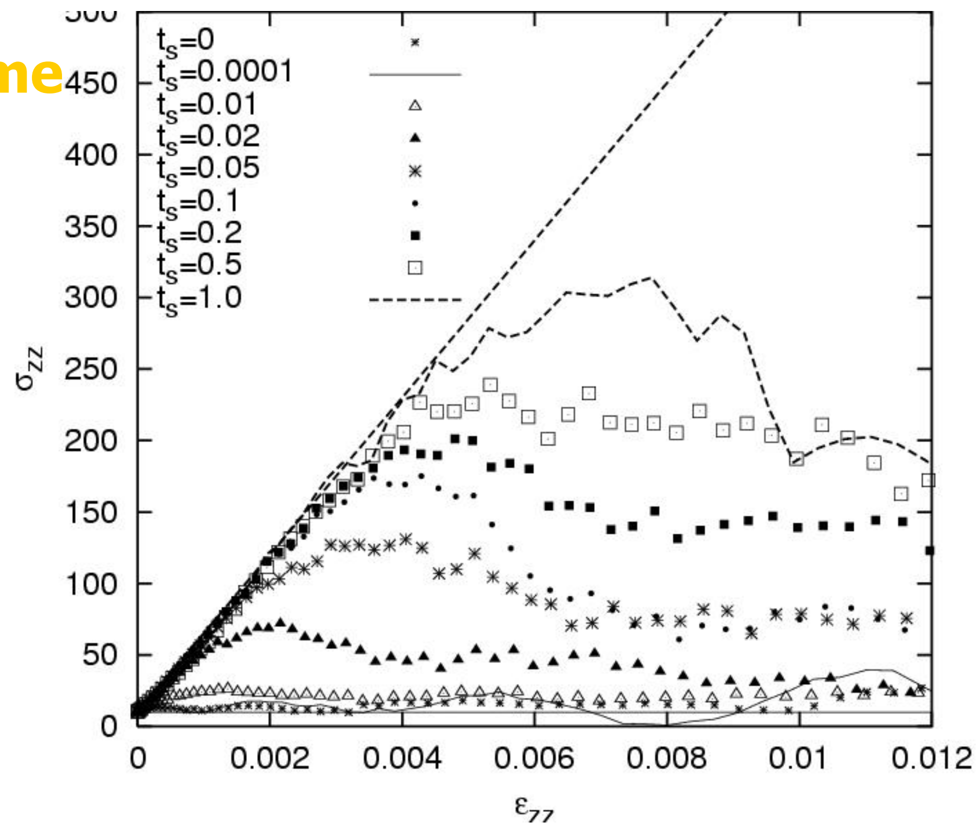


Sintering 6

Stiffness ...



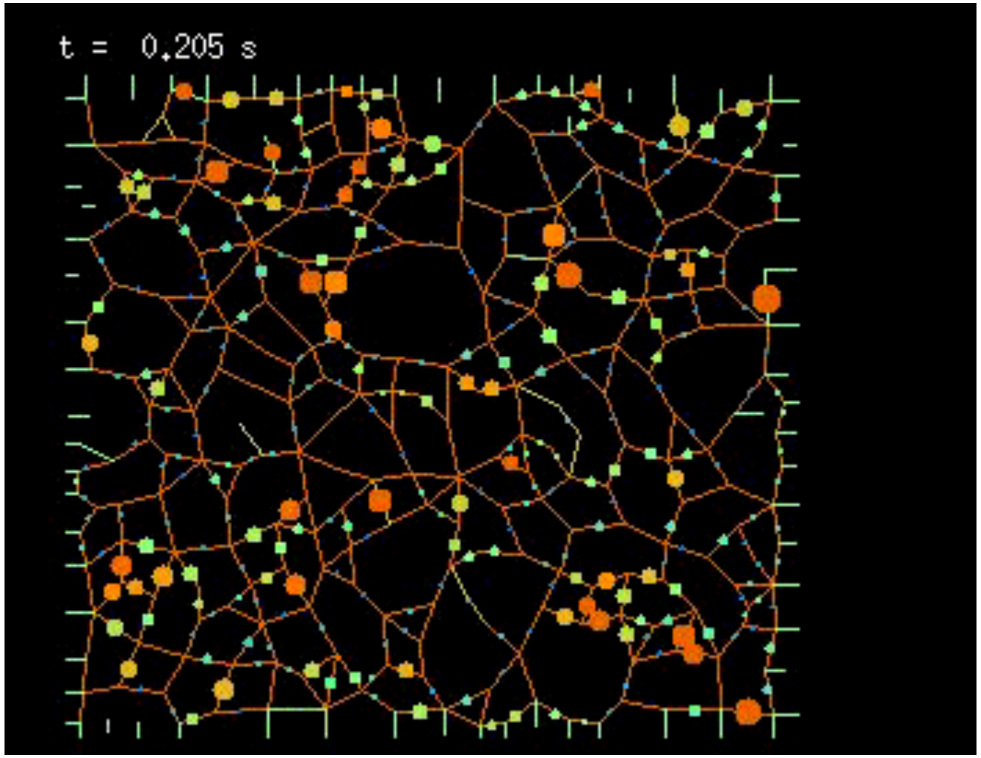
p=100



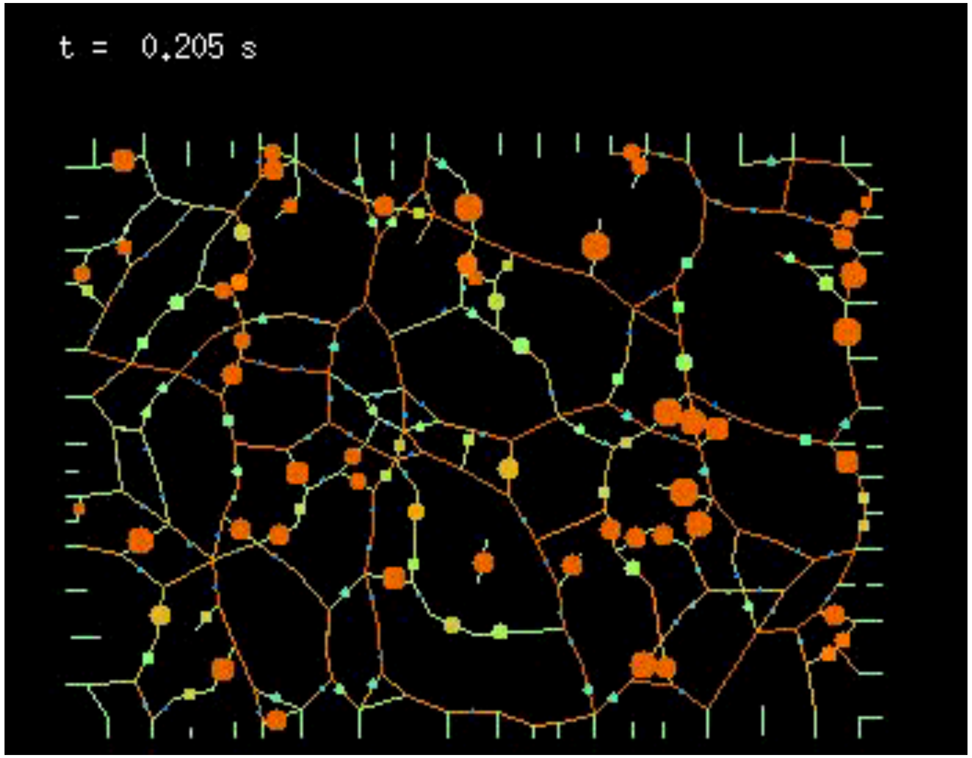
p=10

Sintering

Vibration test



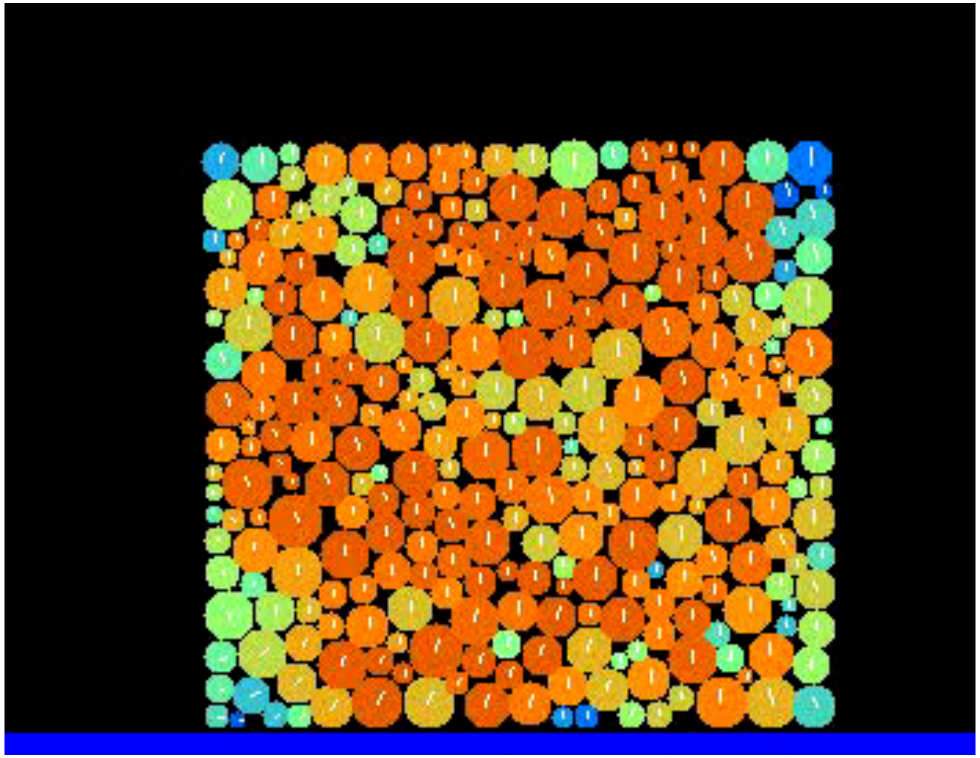
p=100

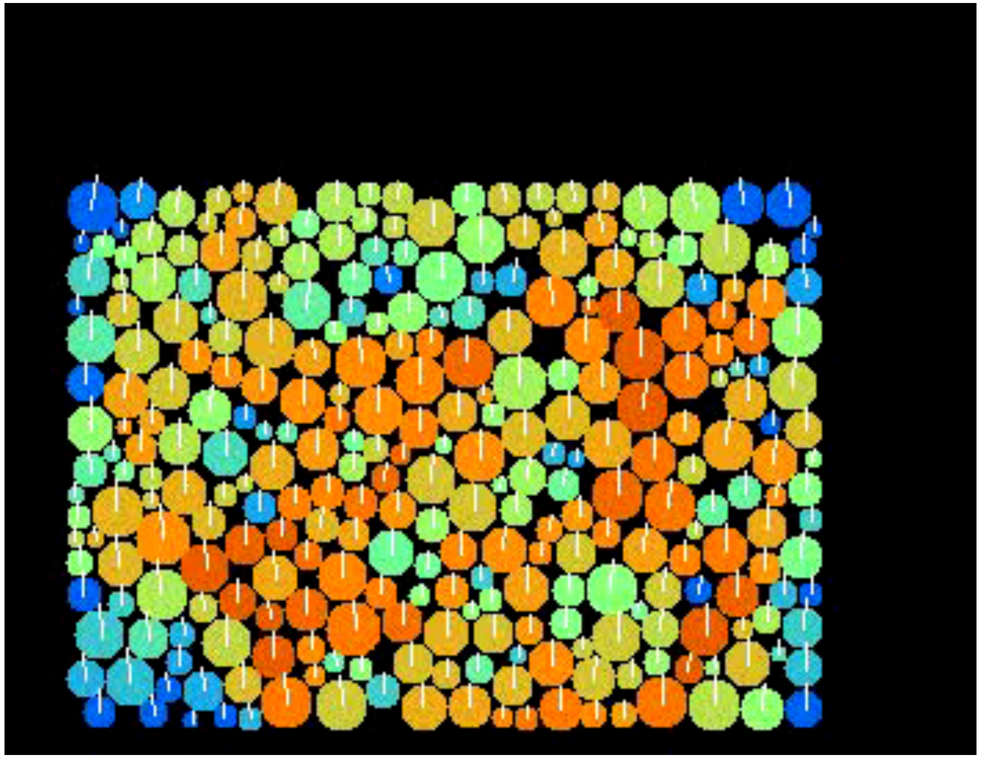


p=10

Sintering (Temperature+Pressure)

Vibration test





p=100

p=10